

Olefin Hydroformylation Products Category

Robust Summaries Environmental Fate and Effects

CAS# 68527-03-7: Pentene, HOF
CAS# 68938-02-3: Pentene, HOF, low-boiling
CAS# 70955-11-2: Hexene, HOF
CAS# 70955-03-2: Hexene, HOF, low-boiling
CAS# 68526-80-7: Alcohols, C6 and C8 iso, distillation residues
CAS# 70955-04-3: Hexene, HOF, high-boiling
CAS# 68527-04-8: Heptene, HOF
CAS# 68526-96-5: Heptene, HOF, low-boiling
CAS# 68526-88-5: Heptene, HOF, high-boiling
CAS# 68527-05-9: Octene, HOF
CAS# 68938-03-4: Octene, HOF, low-boiling
CAS# 68526-89-6: Octene, HOF, high-boiling
CAS# 68938-04-5: Nonene, HOF
CAS# 68526-93-2: Nonene, HOF, low-boiling
CAS# 68526-90-9: Nonene, HOF, high-boiling
CAS# 68516-18-7: Decene, HOF
CAS# 68527-06-0: Dodecene, HOF
CAS# 68526-92-1: Dodecene, HOF, low-boiling
CAS# 68526-91-0: Dodecene, HOF, high-boiling

Revised by:

ExxonMobil Chemical Company

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Robust Summaries - Olefin Hydroformylation Products

Olefin Hydroformylation Products and their corresponding constituents

CAS Number	Product name	Olefin	Alcohol
68527-03-7	Pentene, HOF	C5 (RA)	C6 (68526-79-4)
68938-02-3	Pentene, HOF, low-boiling	C5 (RA)	C6 (68526-79-4)
70955-11-2	Hexene, HOF	C6 (68526-52-3)	C7
70955-03-2	Hexene, HOF, low-boiling	C6 (68526-52-3)	C7 (70914-20-4)
68526-80-7	Alcohols, C6 and C8 is o, distillation residues	-	C6, C8 (68526-79-4) (111-27-3) (104-76-7)
70955-04-3	Hexene, HOF, high-boiling	-	C7-8 (68526-83-0) (104-76-7)
68527-04-8	Heptene, HOF	C7 (68526-53-4)	C8 (68526-83-0) (104-76-7)
68526-96-5	Heptene, HOF, low-boiling	C7 (68526-53-4)	C8 (68526-83-0) (104-76-7)
68526-88-5	Heptene, HOF, high-boiling	-	C8-9 (68526-83-0) (104-76-7)
68527-05-9	Octene, HOF	C8 (68526-54-5)	C9 (68526-84-1) (68515-81-1)
68938-03-4	Octene, HOF, low-boiling	C8 (68526-54-5)	C9 (68526-84-1) (68515-81-1)
68526-89-6	Octene, HOF, high-boiling	-	C9-10 (68526-84-1) (25339-17-7)
68938-04-5	Nonene, HOF	C9 (68526-55-6)	C10 (68526-85-2) (68526-84-1)
68526-93-2	Nonene, HOF, low-boiling	C9 (68526-55-6)	C10 (68526-85-2) (68526-84-1)
68526-90-9	Nonene, HOF, high-boiling	-	C10-11 (68526-85-2) (68526-84-1) (68526-86-3)
68516-18-7	Decene, HOF	C10 (68526-56-7)	C11 (85566-14-9) (68526-86-3) (90604-37-8)
68527-06-0	Dodecene, HOF	C12 (68526-58-9)	C13 (68526-86-3) (112-53-8)
68526-92-1	Dodecene, HOF, low-boiling	C10-12 (68526-58-9)	C13 (68526-86-3) (112-53-8)
68526-91-0	Dodecene, HOF, high-boiling	-	C13-14 (68526-86-3) (112-53-8)

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C6 Alcohol component: Hexanol, branched and linear (68526-79-4)
Fish Acute Toxicity - Flow Through

C7 Alcohol component: Alcohols C6-8, branched (70914-20-4)
Fish Acute Toxicity - Flow Through
Invertebrate Acute Toxicity

C6 Olefin component: Alkenes C6, C6 rich (68526-52-3)
Fish Acute Toxicity
N-Octanol/Water Partition Coefficient

C8 Alcohol component: Alcohols C7-9, branched (68526-83-0)
Fish Acute Toxicity - Flow Through
Invertebrate Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient

C8 Olefin component: Alkenes C7-9, C8 rich (68526-54-5)
Fish Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient

C9 Alcohol component: Alcohols C8-10 iso, C9 rich (68526-84-1)
Fish Acute Toxicity
Invertebrate Acute Toxicity
Algal Toxicity
N-Octanol/Water Partition Coefficient

C10 Alcohol component: Alcohols C9-11 iso, C10 rich (68526-85-2)
Fish Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient

C11 Alcohol component: Alcohols C10-12, C11 rich (90604-37-8)
Fish Acute Toxicity
N-Octanol/Water Partition Coefficient

C10 Olefin component: Alkenes C9-11, C10 rich (68526-56-7)
Fish Acute Toxicity
Manometric Respirometry
N-Octanol/Water Partition Coefficient

C13 Alcohol component: Alcohols C11-14 iso, C13 rich (68526-86-3)
Fish Acute Toxicity
Invertebrate Acute Toxicity
Manometric Respirometry

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N-Octanol/Water Partition Coefficient

C10-C12 Olefin component: Alkenes C12-14, C13 rich (68526-58-9)
Manometric Respirometry

Pentene, HOF (68527-03-7)
Pentene; HOF; low-boiling (68938-02-2)

Fish Acute Toxicity - Calculated
Invertebrate Acute Toxicity - Calculated
Algal Acute Toxicity - Calculated

Hexene; HOF (70955-11-2)
Hexene; HOF; low-boiling (70955-03-2)

Invertebrate Acute Toxicity - Calculated
Algal Acute Toxicity - Calculated

Heptene; HOF (68527-04-8)
Heptene; HOF; low-boiling (68526-96-5)

Fish Acute Toxicity - Calculated
Invertebrate Acute Toxicity - Calculated
Algal Acute Toxicity - Calculated

Octene; HOF (68527-05-9)
Octene; HOF; low-boiling (68938-03-4)

Invertebrate Acute Toxicity - Calculated
Algal Acute Toxicity - Calculated

Nonene; HOF (68938-04-5)
Nonene; HOF; low-boiling (68526-93-2)

Fish Acute Toxicity - Calculated
Invertebrate Acute Toxicity - Calculated
Algal Acute Toxicity - Calculated

Decene; HOF (68516-18-7)

Invertebrate Acute Toxicity - Calculated
Algal Acute Toxicity - Calculated

Category Robust Summary

Water Solubility - Calculated

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Fish Acute Toxicity

Test Substance:	Hexanol branched and linear														
CAS No.	68526-79-4														
Method/Guideline:	No Data														
Year (guideline):	No Data														
Type (test type):	Flow Through Acute Fish Toxicity Test														
GLP:	No Data														
Year (study performed):	1980														
Species:	Fathead Minnow (<i>Pimephales promelas</i>)														
Analytical Monitoring:	Yes														
Exposure Period:	96 hour														
Statistical Method: (FT - ME)	Trimmed Spearman Karber Method														
Test Conditions: (FT - TC)	<p>Treatment solutions were prepared by diluting a 3720mg/L stock solution.</p> <p>Nominal hexanol treatment levels were 41, 68, 113, 189, 315mg/L, which measured 26.7, 49.2, 90.6, 170.0, and 261.5mg/L, respectively.</p> <p>Control/dilution water was EPA Duluth laboratory water.</p> <p>Fifty fish were tested per treatment, divided into two replicates.</p> <p>Treatment volume = 6.3L. Test parameters were as follows: temperature=26.2 Deg C; dissolved oxygen = 6.2mg/L; pH = 7.6; fish age = 28 days old; fish mean wt = 0.117g; fish mean length = 19.7mm; fish loading = 0.464g/L/day.</p> <p>Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.</p>														
• Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.															
Results: (FT - RS)	96 hour LC50 = 97.7 mg/L (95% CI 89.7 to 106) based upon measured values														
Units/Value:															
• Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	<p>Analytical method used was Gas-Liquid Chromatography.</p> <table><tr><th>Measured Conc. (mg/L)</th><th>Fish Total Mortality (@96 hrs)*</th></tr><tr><td>Control</td><td>0</td></tr><tr><td>26.7</td><td>0</td></tr><tr><td>49.2</td><td>0</td></tr><tr><td>90.6</td><td>20</td></tr><tr><td>170.0</td><td>50</td></tr><tr><td>261.5</td><td>50</td></tr></table> <p>* 50 fish added at test initiation</p>	Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*	Control	0	26.7	0	49.2	0	90.6	20	170.0	50	261.5	50
Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*														
Control	0														
26.7	0														
49.2	0														
90.6	20														
170.0	50														
261.5	50														

Robust Summaries - Olefin Hydroformylation Products

Conclusion: (FT - CL)

Reliability: (FT - RL)

(1) Reliable without restriction

Reference: (FT - RE)

Brooke, L. T. et al. 1984. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. I. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.

Other (source): (FT - SO)

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Fish Acute Toxicity

Test Substance:	Alcohols C6-8, branched														
CAS No.	70914-20-4														
Method/Guideline:	No Data														
Year (guideline):	No Data														
Type (test type):	Flow Through Acute Fish Toxicity Test														
GLP:	No Data														
Year (study performed):	1985														
Species:	Fathead Minnow (<i>Pimephales promelas</i>)														
Analytical Monitoring:	Yes														
Exposure Period:	96 hour														
Statistical Method: (FT - ME)	Trimmed Spearman Karber Method														
Test Conditions: (FT - TC)	<p>Treatment solutions were prepared by diluting a 1400mg/L stock solution.</p> <p>Nominal heptanol treatment levels were 12.5, 19.3, 29.7, 45.7, 70.3mg/L, which measured 12.5, 18.1, 28.5, 43.6, and 70.8mg/L, respectively.</p> <p>Control/dilution water was EPA Duluth laboratory water.</p> <p>Twenty fish were tested per treatment. Treatment volume = 2.0L.</p> <p>Test parameters were as follows: temperature=25.6 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 31 days old; fish mean wt = 0.100g; fish mean length = 18.1mm; fish loading = 1.0g/L/day.</p> <p>Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.</p>														
Results: (FT - RS)	96 hour LC50 = 34.5 mg/L (95% CI 33.1 to 36.0) based upon measured values														
Units/Value:	Analytical method used was Gas-Liquid Chromatography.														
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	<table><tr><th>Measured Conc. (mg/L)</th><th>Fish Total Mortality (@96 hrs)*</th></tr><tr><td>Control</td><td>0</td></tr><tr><td>12.5</td><td>0</td></tr><tr><td>18.1</td><td>1</td></tr><tr><td>28.5</td><td>0</td></tr><tr><td>43.6</td><td>20</td></tr><tr><td>70.8</td><td>20</td></tr></table> <p>* 20 fish added at test initiation</p>	Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*	Control	0	12.5	0	18.1	1	28.5	0	43.6	20	70.8	20
Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*														
Control	0														
12.5	0														
18.1	1														
28.5	0														
43.6	20														
70.8	20														

Robust Summaries - Olefin Hydroformylation Products

Conclusion: (FT - CL)

Reliability: (FT - RL)

(1) Reliable without restriction

Reference: (FT - RE)

Geiger, D.L. et al. 1986. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. III. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.

Other (source): (FT - SO)

ExxonMobil Biomedical Sciences, Inc.

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Invertebrate Acute Toxicity

Test Substance:	Alcohol C6-8, branched
CAS No.	70914-20-4
Method/Guideline:	Concept rules of the Dutch Standardization Institute (Adema, 1978)
Type (test type):	Daphnid Acute Toxicity Test
GLP:	No Data
Year (study performed):	1978
Species:	Water Flea (<i>Daphnia magna</i>)
Analytical Monitoring:	No
Exposure Period:	48 hour
Statistical Method:	No Data
Test Conditions:	<p>Tests using 15 different chemicals, including n-Heptanol, were performed at two different laboratories. Lab I was the National Institute of Public Health, Bilthoven, The Netherlands; Lab II was the Central Laboratory, T.N.O., Delft, The Netherlands. The tests were conducted using standardized tests methods proposed by the Dutch Standardization Institute (Adema, 1978). The tests were conducted in duplicate to determine the reproducibility of the results.</p> <p>Organisms were supplied by in-house cultures. Age = <24 hours old.</p>
Results:	48-hour EC50 = 63 mg/L, based upon nominal concentrations of the test chemicals.
Units/Value:	
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	
Conclusion:	Test substance is considered to have moderate acute toxicity
Reliability:	Code 2, Reliable with Restrictions
Reference:	Canton, J.H. and D.M.M. Adema. 1978. Reproducibility of Short-term and Reproduction Toxicity Experiments with <i>Daphnia magna</i> and Comparison of the Sensitivity of <i>Daphnia magna</i> with <i>Daphnia pulex</i> and <i>Daphnia cucullata</i> in Short-term Experiments. <i>Hydrobiologia</i> , 59 :2, pp. 135-140.
Other (reference)	Adema, D.M.M. 1978. <i>Daphnia magna</i> as Test Organism in Acute and Chronic Toxicity Experiments. <i>Hydrobiologia</i> , 59 :2, pp. 125-

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and Chronic Toxicity Experiments. *Hydrobiologia*, **59**:2, pp. 125-134.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

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Fish Acute Toxicity

Test Substance:	Alkenes, C6 Rich
CAS No.	68526-52-3
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Trimmed Spearman-Kärber Method (Hamilton, M.A. <i>et al.</i> 1977. Trimmed Spearman-Kärber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.)

Test Conditions:

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of $\leq 10\%$. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 5 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 6.25, 12.5, 25, 50, and 100 mg/L, which measured 2.9, 6.6, 13.4, 16.9, and 44.0 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.2 mg/L.

Test temperature was 16C (sd = 0.04). Lighting was 623 to 629 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 7.7 to 9.6 mg/L for "new" solutions and 4.5 to 7.5 mg/L for "old" solutions. The pH ranged from 8.2 to 8.5 for "new" solutions and 7.2 to 7.7 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.272 g; mean total length at test termination = 3.5 cm; test loading

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0.272 g; mean total length at test termination = 3.5 cm; test loading = 0.24 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

Results:

Units/Value:

LC50 = 6.6mg/L (CI 5.4 to 8.0), based upon measured concentrations of mean of old and new samples.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was GC-FID

LL50 = 12.8mg/L (CI 10.7 to 15.3), based upon nominal loading levels.

<u>Loading Rate (mg/L)</u>	<u>Measured Conc. (mg/L)</u>	<u>Fish Total Mortality (@96 hrs)*</u>
Control	Control	0
6.25	2.9	0
12.5	6.6	7
25	13.4	15
50	16.9	15
100	44.0	15

* 15 fish added at test initiation

Conclusion:

Reliability:

Code 1, Reliable without Restrictions

Reference:

Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 119058.

Other (source):

American Chemistry Council, Higher Olefins Panel

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Partition Coefficient

Test Substance:	Alkenes, C6 Rich
CAS No.	68526-52-3
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	3.3 - 4.0
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The three major components C8, C9, and C10 alcohols had Log Pow values of 3.3, 3.8, and 4.0, respectively.</p> <p>The retention time for the 3 major components were 6.55, 8.45, and 9.78 minutes, respectively.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	

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Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

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Fish Acute Toxicity

Test Substance:	Alcohols C7-9, branched														
CAS No.	68526-83-0														
Method/Guideline:	No Data														
Year (guideline):	No Data														
Type (test type):	Flow Through Acute Fish Toxicity Test														
GLP:	No Data														
Year (study performed):	1986														
Species:	Fathead Minnow (<i>Pimephales promelas</i>)														
Analytical Monitoring:	Yes														
Exposure Period:	96 hour														
Statistical Method: (FT - ME)	Trimmed Spearman Karber Method														
Test Conditions: (FT - TC)	Treatment solutions were prepared by diluting a 275mg/L stock solution. Nominal octanol treatment levels were 8.6, 10.8, 13.5, 16.9, 21.1mg/L, which measured 8.8, 10.7, 12.7, 16.5, and 20.4mg/L, respectively. Control/dilution water was EPA Duluth laboratory water. Twenty fish were tested per treatment. Treatment volume = 2.0L. Test parameters were as follows: temperature=25.3 Deg C; dissolved oxygen = 7.1mg/L; pH = 7.7; fish age = 28 days old; fish mean wt = 0.075g; fish mean length = 16.5mm; fish loading = 0.75g/L/day. Organism supplier was U.S. EPA Environmental Research Lab, Duluth, MN, USA.														
<ul style="list-style-type: none"> Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading. 															
Results: (FT - RS)	96 hour LC50 = 14.0 mg/L (95% CI 13.6 to 14.5) based upon measured values														
Units/Value:															
<ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method, biological observations, control survival. 	Analytical method used was Gas-Liquid Chromatography. <table> <tr> <th>Measured Conc. (mg/L)</th><th>Fish Total Mortality (@96 hrs)*</th></tr> <tr> <td>Control</td><td>0</td></tr> <tr> <td>8.8</td><td>0</td></tr> <tr> <td>10.7</td><td>1</td></tr> <tr> <td>12.7</td><td>2</td></tr> <tr> <td>16.5</td><td>20</td></tr> <tr> <td>20.4</td><td>20</td></tr> </table>	Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*	Control	0	8.8	0	10.7	1	12.7	2	16.5	20	20.4	20
Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*														
Control	0														
8.8	0														
10.7	1														
12.7	2														
16.5	20														
20.4	20														
	* 20 fish added at test initiation														

Robust Summaries - Olefin Hydroformylation Products

Conclusion: (FT - CL)

Reliability: (FT - RL)

(1) Reliable without restriction

Reference: (FT - RE)

Geiger, D.L. et al. 1988. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. IV. Center for Lake Superior Environmental Studies. University of Wisconsin-Superior, WS, USA.

Other (source): (FT - SO)

ExxonMobil Biomedical Sciences, Inc.

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Invertebrate Acute Toxicity

Test Substance:	Alcohol C7 - 9 branched
CAS No.	68526-83-0
Method/Guideline:	US EPA 660/3-75-009
Type (test type):	Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
GLP:	Unknown
Year (study performed):	1980
Species:	Water Flea (<i>Daphnia magna</i> Straus)
Analytical Monitoring:	No
Exposure Period:	48 hour
Statistical Method:	Spearman-Karber (Finney, D.J., 1971)
Test Conditions:	<p>Individual treatments were prepared by adding varying amounts of test material directly to 250 mL of dilution water in glass beakers. Nominal test concentrations were 10, 18, 32, 56, 100 and 180 mg/L. Four replicates were prepared for each treatment and control. Five daphnids per replicate chamber. Test placed in a temperature-controlled waterbath at 20.5 to 21.0 Deg. C. The test was performed under static conditions.</p> <p>Lighting was 16 hours light : 8 hours dark. Dissolved oxygen ranged from 8.6 to 9.6 mg/L during the study. The pH was ranged from 7.8 to 8.4 during the study. Dilution water hardness was 240 mg/L as CaCO₃, alkalinity was 145 mg/L as CaCO₃, and conductivity was 600 µmhos/cm.</p> <p>Organisms were supplied by in-house cultures. Age = <20 hours old.</p>
Results:	48-hour LC50 = 31.8 mg/L (CI 26.5 - 38.2) as Total Carbon, based upon nominal concentrations.
Units/Value:	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	

Results continued

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<u>Nominal Conc.</u>	<u>% Mortality @ 48 hr.</u>
Control	0
10 mg/L	10
18 mg/L	20
32 mg/L	25
56 mg/L	95
100 mg/L	100
180 mg/L	100

Conclusion:	Test substance is considered to have moderate acute toxicity.
Reliability:	Code 2, Reliable with Restrictions Analytical verification not performed, quality assurance unknown.
Reference:	Union Carbide Corp. (1980). "The Acute Toxicity of MRD-80-4 to the Water Flea (<i>Daphnia magna</i> Straus). Unpublished report.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

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Biodegradation

Test Substance: Alcohols C7-9, branched

CAS No. 68526-83-0

Method/Guideline: OECD 301F, 1992

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1997

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 51 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 82% degradation of the test material was observed. 10% biodegradation was achieved on day 3.

By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	84.7, 77.1, 84.0	82.0
Na Benzoate	91.3, 81.3	86.3

* replicate data

Conclusion: Test substance is considered readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

Robust Summaries - Olefin Hydroformylation Products

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114794A..
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alcohol C7-9, branched
CAS No.	68526-83-0
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	2.9 - 3.4
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The three major components C7, C8, C9 alcohols had Log Pow values of 2.9, 3.0, and 3.4 respectively.</p> <p>The retention time for the 3 major components were 5.72, 6.03, and 7.28 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	
Reliability:	(1) Reliable without restriction

Robust Summaries - Olefin Hydroformylation Products

Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Fish Acute Toxicity

Test Substance:	Alkenes, C7-9, C8 Rich
CAS No.	68526-54-5
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Trimmed Spearman-Kärber Method (Hamilton, M.A. <i>et al.</i> 1977. Trimmed Spearman-Kärber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.)

Test Conditions:

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of $\leq 10\%$. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 2.6, 4.3, 7.2, 12, and 20 mg/L, which measured 0.2, 0.4, 0.7, 1.2, and 2.5 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.2 mg/L.

Test temperature was 15C (sd = 0.09). Lighting was 578 to 580 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.5 to 10.2 mg/L for "new" solutions and 6.5 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.0 to 8.4 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.272 g; mean total length at test termination = 3.5 cm; test loading = 0.24 g of fish/L. The fish were slightly shorter than the guideline

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= 0.24 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

Results:

Units/Value:

LC50 = 0.87mg/L (CI 0.79 to 0.96), based upon measured concentrations of mean of old and new samples.

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Analytical method used was GC-FID

LL50 = 8.9mg/L (CI 9.9 to 13.3), based upon nominal loading levels.

<u>Loading Rate (mg/L)</u>	<u>Measured Conc. (mg/L)</u>	<u>Fish Total Mortality (@96 hrs)*</u>
Control	Control	0
2.6	0.2	0
4.3	0.4	0
7.2	0.7	1
12	1.2	12
20	2.5	12

* 12 fish added at test initiation

Conclusion:

Reliability:

Code 1, Reliable without Restrictions

Reference:

Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 119158.

Other (source):

American Chemistry Council, Higher Olefins Panel

Robust Summaries - Olefin Hydroformylation Products

Biodegradation

Test Substance: Alkenes, C7-9, C8 Rich

CAS No. 68526-54-5

Method/Guideline: OECD 301F, 1993

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1995

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 32 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Approximately 29% biodegradation of the test material was measured on day 28. Approximately 10% biodegradation was achieved on day 17.

By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

% Degradation*	Mean % Degradation	
<u>Sample</u>	<u>(day 28)</u>	<u>(day 28)</u>
Test Material	44.1, 28.6, 15.0	29.2
Na Benzoate	98.9, 95.5	97.2

* replicate data

Conclusion:

Reliability: Code 1, Reliable without Restrictions

Robust Summaries - Olefin Hydroformylation Products

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 119194A..
Other (source):	American Chemistry Council, Higher Olefins Panel

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alkenes, C7-9, C8 Rich
CAS No.	68526-54-5
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	4.2 - 5.1
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The five major components C10 to C12 alcohols had Log Pow values of 4.2 to 5.1.</p> <p>The retention time for the 8 major components were 10.72 to 20.35 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	

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Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Fish Acute Toxicity

Test Substance:	Alcohol C8 - 10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Bionomial Method
Test Conditions:	<p>Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of $\leq 10\%$ of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.</p> <p>Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 572 to 573 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.0 mg/L and from 4.8 to 6.3 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.8 to 8.5 during the study. Fish were not fed during the study.</p> <p>Fish Mean Wt.= 0.361g. Mean Total length = 3.8cm, Test Loading = 0.40 g of fish/L.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	
Results:	LC50 = 10.1mg/L (CI 7.3 to 14.1), based upon measured concentrations of mean of old and new samples.
Units/Value:	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was GC-FID
	LL50 = 11.2 mg/L (CI 7.5 to 16.6), based upon nominal loading levels.
Results continued	

Robust Summaries - Olefin Hydroformylation Products

<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.</u>
Control	Below detection	0
0.7 mg/L	1.7 mg/L	0
1.5 mg/L	1.9 mg/L	0
3.3 mg/L	3.9 mg/L	0
7.5 mg/L	7.3 mg/L	0
16.6 mg/L	14.1 mg/L	100

Dissolved oxygen levels dropped below 60% of saturation in some of the treatments on Days 1 through 4 of the test. Since no mortality occurred in these treatments, the deviations are not believed to have affected the outcome of the study.

Conclusion:

Test substance is considered to have moderate acute toxicity

Reliability:

Code 1, Reliable without Restrictions

Reference:

Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 114858.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Invertebrate Acute Toxicity

Test Substance:	Alcohol C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	OECD 202 Daphnia sp. Acute Immobilization Test
Type (test type):	Daphnid Acute Toxicity Test
GLP:	Yes
Year (study performed):	1996
Species:	Water Flea (<i>Daphnia magna</i>)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions:	<p>Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added to 2.0L of dilution water in a 2L glass aspirator bottle. The solutions were mixed for 25 hours at a vortex of $\leq 20\%$ of the total depth. The test solutions were removed through the outlet at the bottom of each mixing vessel into four replicates of 140 mL in 125 mL glass erlenmeyer flasks (no headspace). Five daphnids were added to each test replicate and the replicates sealed. The test was performed under static conditions with no aeration.</p> <p>Test temperature was 21.4 Deg C., Lighting was 16 hours light : 8 hours dark with 638 to 639 Lux during full daylight periods. Dissolved oxygen ranged from 7.3 to 8.2 mg/L during the study. The pH was ranged from 7.7 to 8.4 during the study.</p> <p>Organisms were supplied by in-house cultures. Age = <24 hours old, from 13 and 16-day old parents.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.	
Results:	48-hour EC50 = 4.9 mg/L (CI 4.5 - 5.4), based upon measured concentrations of mean of old and new samples.
Units/Value:	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was Total Organic Carbon (TOC).

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Results continued	<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Immobilization @ 24 hr.</u>
	Control	0	0
	1.56 mg/L	0.80 mg/L	0
	3.12 mg/L	1.82 mg/L	0
	6.25 mg/L	3.05 mg/L	0
	12.5 mg/L	4.39 mg/L	40
	25.0 mg/L	6.14 mg/L	85

Conclusion: Test substance is considered to have moderate acute toxicity

Reliability: Code 1, Reliable without Restrictions

Reference: Exxon Biomedical Sciences, Inc. Acute Toxicity for Daphnia, 149542.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Algal Toxicity

Test Substance:	Alcohol C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	7-Day Cell Multiplication Inhibition Test
Type (test type):	Static Toxicity Test
GLP:	No Data
Year (study performed):	No Data
Species/Strain:	Green Alga (<i>Scenedesmus quadricauda</i>)
Analytical Monitoring:	No
Exposure Period:	7 days
Statistical Method:	None applied. The toxicity threshold (TT) was determined graphically by plotting the highest non-toxic concentration versus its mean extinction value against the lowest toxic concentration versus its mean extinction value and calculating the toxicant concentration at 3% below the no effect level.
Test Conditions:	<p>Treatment solutions were prepared by diluting a stock isooctanol solution. Testing was conducted in metal capped, 300 ml Erlenmeyer flasks containing 50 ml of treatment solution. Treatment solutions contained isooctanol, cells, double distilled water, and a sterile, defined nutrient medium. The control solution contained nutrient medium, to which sterile double distilled water was added. Growth inhibition measurements were only determined on day 7.</p> <p>Cell growth was determined by using a turbidimetric procedure that measured primary light extinction (monochromatic radiation at 578 nm) through a cell suspension of 10 mm thickness.</p>
Results:	
Units/Value:	7-day TT (toxicity threshold) for growth = 8.5 mg/L based on nominal values
Measurement (cells/growth)	<p>The TT value for growth is calculated by identifying the treatment level that is greater or equal to 3% below the treatment level that did not exhibit toxic effects as measured by the extinction of primary light of monochromatic radiation at 578 nm.</p>
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	
Conclusion:	

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Reliability:

(2) Reliable with restrictions

Although a non-standardized method was described in the article, data were not provided on the test parameters, replication, or results from individual treatment and control solutions. This lack of information supports a reliability rating of 2.

Reference:

Bringmann, G. and R. Kuhn. 1980. Comparison of the Toxicity Thresholds of Water Pollutants to Bacteria, Algae, and Protozoa in the Cell Multiplication Inhibition Test. *Water Research*. 14:231-241.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alcohol C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	3.4 - 3.9
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The three major components C8, C9, C10 alcohols had Log Pow values of 3.4, 3.8, and 3.9 respectively.</p> <p>The retention time for the 3 major components were 6.91, 8.42, and 8.96 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	
Reliability:	(1) Reliable without restriction

Robust Summaries - Olefin Hydroformylation Products

Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Fish Acute Toxicity

Test Substance:	Alcohol C9 - 11 iso, C10 rich
CAS No.	68526-85-2
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions:	<p>Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19.5L of dilution water in a 20L glass carboy. The carboys were covered with an opaque covering to prevent photochemical degradation of the soluble components. The solutions were mixed for 24 hours at a vortex of $\leq 10\%$ of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.</p> <p>Test temperature was 15.0 Deg C., Lighting was 16 hours light : 8 hours dark with 569 to 572 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 9.9 mg/L and from 5.7 to 7.6 mg/L in "old" solutions prior to renewals. The pH was ranged from 7.0 to 8.5 during the study. Fish were not fed during the study.</p> <p>Fish Mean Wt.= 0.185g. Mean Total length = 3.0cm, Test Loading = 0.21 g of fish/L.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	
Results:	LC50 = 3.1mg/L (CI 2.4 to 4.0), based upon measured concentrations of mean of old and new samples.
Units/Value:	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	<p>Analytical method used was GC-FID</p> <p>LL50 = 3.0 mg/L (Could not calculate CI), based upon nominal loading levels.</p>
Results continued	

Robust Summaries - Olefin Hydroformylation Products

<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.</u>
Control	Below detection	7
1.2 mg/L	1.2 mg/L	13
2.5 mg/L	2.4 mg/L	13
5 mg/L	5.2 mg/L	100
10 mg/L	9.9 mg/L	100
20 mg/L	19.5 mg/L	100

Dissolved oxygen levels dropped below 60% (57%) of saturation in the 2.4 mg/L treatment on Days 3 and 4 of the test. Since only 13% mortality occurred at this level, and the solutions were renewed daily, this drop in DO did not affect the outcome of the study.

Conclusion:	Test substance is considered to have moderate acute toxicity
Reliability:	Code 1, Reliable without Restrictions
Reference:	Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 114958.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Biodegradation

Test Substance: Alcohol C9 - 11 iso, C10 rich

CAS No. 68526-85-2

Method/Guideline: OECD 301F, 1992

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1997

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 43 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was readily biodegradable. Half-life was reached by day 11. By day 28, 71.1% degradation of the test material was observed. 10% biodegradation was achieved on day 4.

By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	74.0, 72.6, 66.5	71.1
Na Benzoate	91.3, 81.3	86.3

* replicate data

Conclusion: Test substance is considered readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

Robust Summaries - Olefin Hydroformylation Products

Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 114994A..
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alcohol C9 - 11 iso, C10 rich
CAS No.	68526-85-2
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	3.8
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
<ul style="list-style-type: none">Note: Concentration prep., vessel type, replication, test conditions.	
Results:	
Units/Value:	<p>The test substance eluted as several groups. The two major components C9, C10 alcohols had Log Pow values of 3.8.</p> <p>The retention time for the 2 major components were 8.37, and 8.74 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method.	
Conclusion:	
Reliability:	(1) Reliable without restriction

Robust Summaries - Olefin Hydroformylation Products

Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Fish Acute Toxicity

Test Substance:	Alcohol C10 - 12, C11 rich
CAS No.	90604-37-8
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Probit procedure of SAS (Finney, 1971)
Test Conditions:	<p>Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19.5L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of $\leq 10\%$ of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.</p> <p>Test temperature was 15 Deg C., Lighting was 16 hours light : 8 hours dark with 572 to 573 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.4 to 10.0 mg/L and from 4.8 to 6.4 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.8 to 8.6 during the study. Fish were not fed during the study.</p> <p>Fish Mean Wt.= 0.365g. Mean Total length = 3.6cm, Test Loading = 0.40 g of fish/L.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	
Results:	LC50 = 1.8 mg/L (CI 1.4 to 2.5), based upon measured concentrations of mean of old and new samples.
Units/Value:	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was GC-MSD LL50 = 2.1 mg/L (CI 1.7 to 2.8), based upon nominal loading levels.
Results continued	

Robust Summaries - Olefin Hydroformylation Products

<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.</u>
Control	Below detection	0
0.3 mg/L	0.48 mg/L	13
0.5 mg/L	0.52 mg/L	0
1.4 mg/L	1.1 mg/L	0
3.5 mg/L	3.1 mg/L	100
8.8 mg/L	7.2 mg/L	100

Dissolved oxygen levels dropped below 60% (40-60%) of saturation in some of the treatments on Days 1 through 4 of the test. Based on mortality observations, these deviations are not believed to have affected the outcome of the study.

Conclusion:	Test substance is considered to have moderate acute toxicity
Reliability:	Code 1, Reliable without Restrictions
Reference:	Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118458.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alcohol C10 - 12, C11 rich
CAS No.	90604-37-8
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	3.9 - 4.3
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The three major components C9, C10, C11 alcohols had Log Pow values of 3.9, 4.2, and 4.3 respectively.</p> <p>The retention time for the 3 major components were 9.01, 10.86, and 11.88 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	

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Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

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Fish Acute Toxicity

Test Substance:	Alkenes, C9-11, C10 Rich
CAS No.	68526-56-7
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1995
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Trimmed Spearman-Kärber Method (Hamilton, M.A. <i>et al.</i> 1977. Trimmed Spearman-Kärber Method for Estimating Median Lethal Concentration in Toxicity Bioassays. Environ. Sci. Technol. 11:714-719.)

Test Conditions:

- **Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**

Each test solution was prepared by adding the test substance, via syringe, to 19.5 L of laboratory blend water in 20 L glass carboys. The solutions were mixed for 24 hours with a vortex of $\leq 10\%$. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22°C). After mixing, the solutions were allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 4 fish were added. Three replicates of each test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

Test material loading levels included: 0.2, 0.4, 1.2, 3.5, and 10 mg/L, which measured 0.01, 0.03, 0.06, 0.08, and 2.6 mg/L, respectively, and are based on the mean of samples taken from the new and old test solutions. A control containing no test material was included and the analytical results were below the quantitation limit, which was 0.03 mg/L.

Test temperature was 16°C (sd = 0.2). Lighting was 445 to 555 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 8.7 to 9.9 mg/L for "new" solutions and 7.2 to 8.5 mg/L for "old" solutions. The pH ranged from 7.0 to 8.8 for "new" solutions and 7.3 to 8.7 for "old" solutions.

Fish supplied by Thomas Fish Co. Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.175 g; mean total length at test termination = 3.0 cm; test loading

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0.175 g; mean total length at test termination = 3.0 cm; test loading = 0.19 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

Results:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

96-hour LL50 = 4.8 mg/L (95% CI 3.8 to 6.0 mg/L) based upon loading rates.

96-hour LC50 = 0.12 mg/L (95% CI 0.11 to 0.14 mg/L) based upon measured values of old and new solutions.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

Results continued

<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.*</u>
Control	Control	0
0.2 mg/L	0.01 mg/L	0
0.4 mg/L	0.03 mg/L	0
1.2 mg/L	0.06 mg/L	0
3.5 mg/L	0.08 mg/L	3
10.0 mg/L	0.26 mg/L	15**

* 15 fish added at test initiation

** 1 mortality not test related

Conclusion:

Reliability:

Code 1, Reliable without Restrictions

Reference:

Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 119258.

Other (source):

American Chemistry Council, Higher Olefins Panel

Robust Summaries - Olefin Hydroformylation Products

Biodegradation

Test Substance: Alkenes, C9-11, C10 Rich

CAS No. 68526-56-7

Method/Guideline: OECD 301F, 1993

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1995

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 42 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was not readily biodegradable. Approximately 21% biodegradation of the test material was measured on day 28.

Approximately 10% biodegradation was achieved on Day 17. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	20.9, 19.9, 22.6	21.1
Na Benzoate	98.9,95.5	97.2

* replicate data

Conclusion: Test substance is considered not readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

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Reference: Exxon Biomedical Sciences, Inc. 1997. Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119294A.

Other (source): American Chemistry Council, Higher Olefins Panel

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alkenes, C9-11, C10 Rich
CAS No.	68526-56-7
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	4.9 - 5.8
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The eight major components C11 to C13 alcohols had Log Pow values of 4.9 to 5.8.</p> <p>The retention time for the 8 major components were 18.16 to 36.55 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	

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Reliability:	(1) Reliable without restriction
Reference:	Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Fish Acute Toxicity

Test Substance:	Alcohol C11 - 14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 203 Fish Acute Toxicity Test
Type (test type):	Fish Acute Toxicity Test
GLP:	Yes
Year (study performed):	1998
Species:	Rainbow Trout (<i>Oncorhynchus mykiss</i>)
Analytical Monitoring:	Yes
Exposure Period:	96 hour
Statistical Method:	Spearman-Karber Method (Hamilton, et al, 1977)
Test Conditions:	<p>Individual Water Accomodated Fractions (WAF's) were prepared for each test treatment. The test substance was added volumetrically, via a syringe, to 19L of dilution water in a 20L glass carboy. The solutions were mixed for 24 hours at a vortex of $\leq 10\%$ of the total depth. The test solutions were pumped from each mixing vessel into three replicates of 4.5L in 4.0L glass aspirator bottles (no headspace). Five fish were added to each test replicate and the replicates sealed. Daily renewals were performed by removing ~80% of the test solution through the port at the bottom and refilling with fresh solution.</p> <p>Test temperature was 13.8 Deg C., Lighting was 16 hours light : 8 hours dark with 551 to 736 Lux during full daylight periods. Dissolved Oxygen at initiation ranged from 8.3 to 9.2 mg/L and from 6.6 to 8.8 mg/L in "old" solutions prior to renewals. The pH was ranged from 6.6 to 8.2 during the study. Fish were not fed during the study.</p> <p>Fish Mean Wt.= 0.131g. Mean Total length = 2.7cm, Test Loading = 0.15 g of fish/L.</p>
<ul style="list-style-type: none">Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	
Results:	LC50 = 0.42 mg/L (CI 0.37 to 0.48), based upon measured concentrations of mean of old and new samples.
Units/Value:	
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	<p>Analytical method used was GC-MSD</p> <p>LL50 = 0.64 mg/L (CI 0.57 to 0.73), based upon nominal loading levels.</p>

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Results continued

<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 96 hr.</u>
Control	Below detection	0
0.25 mg/L	0.17 mg/L	0
0.5 mg/L	0.32 mg/L	13
1.0 mg/L	0.67 mg/L	100
2.0 mg/L	0.94 mg/L	100
5.0 mg/L	0.93 mg/L	100

Conclusion:	Test substance is considered to have high acute toxicity
Reliability:	Code 1, Reliable without Restrictions
Reference:	Exxon Biomedical Sciences, Inc. Fish Acute Toxicity Test, 118358A.
Other (source):	ExxonMobil Biomedical Sciences, Inc.

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Invertebrate Acute Toxicity

Test Substance:	Alcohol C11 - 14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	US EPA TSCA 797.1300
Type (test type):	Daphnid Acute Toxicity Test
GLP:	Unknown
Year (study performed):	1986
Species:	Water Flea (<i>Daphnia magna</i>)
Analytical Monitoring:	Yes
Exposure Period:	48 hour
Statistical Method:	Probit procedure based on Litchfield-Wilcoxon (1949)
Test Conditions:	<p>The water soluble fraction (WSF) was prepared by combining the test substance with dilution water at a ratio of 1:150. The solutions were mixed for 96 hours and allowed to settle for 1 hour prior to use as the 100% WSF stock solution. Test solutions were prepared by diluting the 100% WSF stock. Two replicates of 250 mL in 400 mL autoclaved glass beakers were prepared at each treatment level. Ten daphnids per replicate chamber. Test chambers were covered with glass and placed in a temperature-controlled waterbath. The test was performed under static conditions.</p> <p>Test temperature was 20.8 Deg C., Lighting was 16 hours light : 8 hours dark with 57.5 to 67.3 footcandles during full daylight periods. Dissolved oxygen ranged from 8.1 to 9.1 mg/L during the study. The pH was ranged from 7.8 to 8.2 during the study. Dilution water hardness was 130 mg/L as CaCO₃.</p> <p>Organisms were supplied by in-house cultures. Age = <24 hours old from 19-day old parents.</p>
Results:	
Units/Value:	<p>48-hour LC50 = 0.71 mg/L (CI 0.59 - 0.85) as Total Carbon, based upon mean measured concentrations of Day 0 and Day 2 samples. 48-hour LC50 value equivalent to 16.7% WSF.</p>
<ul style="list-style-type: none">Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.	Analytical method used was Total Carbon

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Results continued	<u>Nominal Conc.</u>	<u>Measured Conc.</u>	<u>% Mortality @ 48 hr.</u>
	Control	-	0
	6.25% WSF	0.28 mg/L	0
	12.5% WSF	0.58 mg/L	30
	25% WSF	1.03 mg/L	85
	50% WSF	1.85 mg/L	100
	100% WSF	4.17 mg/L	100

Conclusion: Test substance is considered to have high acute toxicity.

Reliability: Code 2, Reliable with Restrictions

Analytical verification not test substance specific, quality assurance unknown.

Reference: Exxon Biomedical Sciences, Inc. Static Acute Daphnia Toxicity Test, 269342.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Biodegradation

Test Substance: Alcohol C11 - 14 iso, C13 rich

CAS No. 68526-86-3

Method/Guideline: OECD 301F, 1992

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1998

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 57 mg/L. Sodium benzoate (positive control) concentration was 44mg/L.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was not readily biodegradable. Half-life was reached by day 25. By day 28, 58.1% degradation of the test material was observed. 10% biodegradation was achieved on day 7.

By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

<u>Sample</u>	<u>% Degradation*</u> <u>(day 28)</u>	<u>Mean % Degradation</u> <u>(day 28)</u>
Test Material	60.1, 60.7, 53.7	58.1
Na Benzoate	87.1, 85.4	86.2

* replicate data

Conclusion: Test substance is considered not readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

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Reference:	Exxon Biomedical Sciences Inc., Ready Biodegradability : OECD 301F Manometric Respirometry Test. 180294A..
Other (source):	ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Partition Coefficient

Test Substance:	Alcohol C11 - 14 iso, C13 rich
CAS No.	68526-86-3
Method/Guideline:	OECD 117
Year (guideline):	1989
Type (test type):	N-Octanol/Water Partition Coefficient (HPLC method)
GLP:	Yes
Year (study performed):	1998
Temperature:	~30 Deg C
Log Pow Value:	4.2 - 5.0
Test Conditions:	<p>The test substance was evaluated as a solution in HPLC grade methanol. Six reference compounds were also evaluated in a standard combined reference solution (2-butanone, acetophenone, naphthalene, biphenyl, n-butylbenzene, and 4,4-DDT) in 75% methanol and 25% distilled water. The pH of the solution was 5.4.</p> <p>Two customized alcohol reference solutions were also prepared containing five of the ten alcohol compounds (1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, 1-decanol, 1-undecanol, 1-dodecanol, 1-tridecanol, 1-tetradecanol, 1-pentadecanol) in 87.5% methanol and 12.5% distilled water. The pH of both solutions was 7.3.</p> <p>The pH of the evaluated solutions was the same as the reference solution it was evaluated against.</p> <p>The test substance was analyzed against a Standard Log Pow Reference Compound Solution and a customized Alcohol Reference Compound Solution. Only the peaks detected by refractive index (RI) were reported.</p>
Results:	
Units/Value:	<p>The test substance eluted as several groups. The five major components C9, C10, C11, C12, C13 alcohols had Log Pow values of 4.2, 4.4, 4.5, 4.7, and 5.0 respectively.</p> <p>The retention time for the 4 major components were 11.04, 12.02, 13.53, 14.69, and 18.40 minutes.</p> <p>All values were measured using High Performance Liquid Chromatography (HPLC).</p>
Conclusion:	
Reliability:	(1) Reliable without restriction

Robust Summaries - Olefin Hydroformylation Products

Reference: Exxon Biomedical Sciences Inc. 1998. N-Octanol/Water Partition Coefficient. Study #193387D.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Biodegradation

Test Substance: Alkenes, C12-14, C13 Rich

CAS No. 68526-58-9

Method/Guideline: OECD 301F, 1993

Type (test type): Manometric Respirometry Test

GLP: Yes

Year (study performed): 1995

Inoculum: Domestic activated sludge

Exposure Period: 28 days

Test Conditions:

- Note: Concentration prep. vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, loading.**

Non acclimated activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (Phosphate buffer, Ferric chloride, Magnesium sulfate, Calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material concentration was approximately 45 mg/L. Sodium benzoate (positive control) concentration was 50mg/L.

Test temperature was 22 +/- 1 Deg C.

All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Test material was not readily biodegradable. Approximately 8% biodegradation of the test material was measured on day 28. By day 14, >60% biodegradation of positive control was observed, which met the guideline requirement. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

	% Degradation*	Mean % Degradation
<u>Sample</u>	<u>(day 28)</u>	<u>(day 28)</u>
Test Material	6.28, 8.26, 8.35	7.63
Na Benzoate	88.2, 86.5	87.4

* replicate data

Conclusion: Test substance is considered not readily biodegradable.

Reliability: Code 1, Reliable without Restrictions

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Reference: Exxon Biomedical Sciences, Inc. 1997. Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119394A.

Other (source): American Chemistry Council, Higher Olefins Panel

Robust Summaries - Olefin Hydroformylation Products

Calculated Fish Acute Toxicity

Test Substance:	Other TS [CAS # 68527-03-7; 68938-02-3]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Fish Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Fish (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-03-7; 68938-02-3, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C5 Olefin	2.66
C6 Alcohol	1.82

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated fish acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-03-7; 68938-02-3 are as follows:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	<u>Fish Acute 96-hr LC50 (mg/L)</u> (Estimated)	(Measured)
C5 Olefin	2.66	12.5	nt
C6 Alcohol	1.82	111.8	97.7

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

68527-03-7 Pentene, HOF
68938-02-3 Pentene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit a fish 96-hour LC50 value of 12.5 mg/L, while the alcohol fraction would be expected to exhibit an LC50 value of 111.8 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater fish at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Invertebrate Acute Toxicity

Test Substance:	Other TS [CAS # 68527-03-7; 68938-02-3]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Invertebrate (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-03-7; 68938-02-3, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C5 Olefin	2.66
C6 Alcohol	1.82

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated invertebrate acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-03-7; 68938-02-3 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Daphnid Acute <u>48-hr EC50 (mg/L)</u>
C5 Olefin	2.66	14.0
C6 Alcohol	1.82	118.3

Test Substance:

68527-03-7 Pentene, HOF
68938-02-3 Pentene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an invertebrate 48-hour EC50 value of 14.0 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 118.3 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater invertebrates at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Reference:

Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Acute Alga Toxicity

Test Substance:	Other TS [CAS # 68527-03-7; 68938-02-3]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Algae (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-03-7; 68938-02-3, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C5 Olefin	2.66
C6 Alcohol	1.82

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated alga acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-03-7; 68938-02-3 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Alga Acute <u>96-hr EC50 (mg/L)</u>
C5 Olefin	2.66	9.1
C6 Alcohol	1.82	73.2

Test Substance:

68527-03-7 Pentene, HOF
68938-02-3 Pentene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an alga 96-hour EC50 value of 9.1 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 73.2 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater green algae at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Reference:

Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Invertebrate Acute Toxicity

Test Substance:	Other TS [CAS # 70955-11-2; 70955-03-2]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Invertebrate (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 70955-11-2; 70955-03-2, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C6 Olefin	3.15
C7 Alcohol	2.31

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated invertebrate acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 70955-11-2; 70955-03-2 are as follows:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	<u>Calculated log K_{ow}</u>	<u>Daphnia Acute 48-hr EC50 (mg/L) Estimated</u>	<u>Measured</u>
C5 Olefin	3.15	6.0	nt
C6 Alcohol	2.31	48.2	63.0

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

70955-11-3 Hexene, HOF
70955-03-2 Hexene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an invertebrate 48-hour EC50 value of 6.0 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 48.2 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater invertebrates at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Acute Alga Toxicity

Test Substance:	Other TS [CAS # 70955-11-2; 70955-03-2]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Algae (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). The following chemicals are representative of the substances associated with CAS #'s 70955-11-2; 70955-03-2, which are complex, multi-constituent substances.
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C6 Olefin	3.15
C7 Alcohol	2.31

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated alga acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 70955-11-2; 70955-03-2 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Alga Acute <u>96-hr EC50 (mg/L)</u>
C6 Olefin	3.15	4.0
C7 Alcohol	2.31	30.7

Test Substance:

70955-11-2 Hexene, HOF
70955-03-2 Hexene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an alga 96-hour EC50 value of 4.0 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 30.7 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater green algae at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Reference:

Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Fish Acute Toxicity

Test Substance:	Other TS [CAS # 68527-04-8; 68526-96-5]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Fish Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Fish (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). The following chemicals are representative of the substances associated with CAS #'s 68527-04-8; 68526-96-5, which are complex, multi-constituent substances.
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C7 Olefin	3.64
C8 Alcohol	2.81

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated fish acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-04-8; 68526-96-5 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Fish Acute 96-hr LC50 (mg/L) <u>Estimated</u>	<u>Measured</u>
C7 Olefin	3.64	2.1	nt
C8 Alcohol	2.81	16.7	14.0

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

68527-04-8 Heptene, HOF
68526-96-5 Heptene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit a fish 96-hour LC50 value of 2.1 mg/L, while the alcohol fraction would be expected to exhibit an LC50 value of 16.7 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater fish at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Invertebrate Acute Toxicity

Test Substance:	Other TS [CAS # 68527-04-8; 68526-96-5]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Invertebrate (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-04-8; 68526-96-5, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C7 Olefin	3.64
C8 Alcohol	2.81

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated invertebrate acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-04-8; 68526-96-5 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	<u>Calculated log K_{ow}</u>	<u>Daphnia Acute 48-hr LC50 (mg/L) Estimated</u>	<u>Measured</u>
C7 Olefin	3.64	2.5	nt
C8 Alcohol	2.81	19.0	31.8

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

68527-04-8 Heptene, HOF
68526-96-5 Heptene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an invertebrate 48-hour EC50 value of 2.5 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 19.0 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater invertebrates at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Acute Alga Toxicity

Test Substance:	Other TS [CAS # 68527-04-8; 68526-96-5]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Algae (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-04-8; 68526-96-5, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C7 Olefin	3.64
C8 Alcohol	2.81

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated alga acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-04-8; 68526-96-5 are as follows:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Alga Acute <u>96-hr EC50 (mg/L)</u>
C7 Olefin	3.64	1.7
C8 Alcohol	2.81	12.4

Test Substance:

68527-04-8 Heptene, HOF
68526-96-5 Heptene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an alga 96-hour EC50 value of 1.7 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 12.4 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater green algae at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Reference:

Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Invertebrate Acute Toxicity

Test Substance:	Other TS [CAS # 68527-05-9; 68938-03-4]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Invertebrate (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-05-9; 68938-03-4, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C8 Olefin	4.13
C9 Alcohol	3.30

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated invertebrate acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-05-9; 68938-03-4 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	<u>Calculated log K_{ow}</u>	<u>Daphnia Acute 48-hr LC50 (mg/L) Estimated</u>	<u>Measured</u>
C8 Olefin	4.13	1.0	nt
C9 Alcohol	3.30	7.5	4.9

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

68527-05-9 Octene, HOF
68938-03-4 Octene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an invertebrate 48-hour EC50 value of 1.0 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 7.5 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater invertebrates at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Acute Alga Toxicity

Test Substance:	Other TS [CAS # 68527-05-9; 68938-03-4]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Algae (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68527-05-9; 68938-03-4, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C8 Olefin	4.13
C9 Alcohol	3.30

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated alga acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68527-05-9; 68938-03-4 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Alga Acute 96-hr LC50 (mg/L) <u>Estimated</u>	<u>Measured</u>
C8 Olefin	4.13	0.7	nt
C9 Alcohol	3.30	5.1	8.5

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

68527-05-9 Octene, HOF
68938-03-4 Octene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an alga 96-hour EC50 value of 0.7 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 5.1 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater green algae at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Fish Acute Toxicity

Test Substance:	Other TS [CAS # 68938-04-5; 68526-93-2]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Fish Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Fish (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68938-04-5; 68526-93-2, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C9 Olefin	4.62
C10 Alcohol	3.79

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated fish acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68938-04-5; 68526-93-2 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Fish Acute 96-hr LC50 (mg/L) <u>Estimated</u>	<u>Measured</u>
C9 Olefin	4.62	0.32	nt
C10 Alcohol	3.79	2.4	3.1

nt = not tested

The measured value is based on toxicity testing and supports the use of the ECOSAR model to calculate toxicity values for component chemicals of these substances.

Test Substance:

68938-04-5 Nonene, HOF
68526-93-2 Nonene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit a fish 96-hour LC50 value of 0.32 mg/L, while the alcohol fraction would be expected to exhibit an LC50 value of 2.4 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater fish at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Robust Summaries - Olefin Hydroformylation Products

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Invertebrate Acute Toxicity

Test Substance:	Other TS [CAS # 68938-04-5; 68526-93-2]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Invertebrate (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68938-04-5; 68526-93-2, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C9 Olefin	4.62
C10 Alcohol	3.79

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated invertebrate acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68938-04-5; 68526-93-2 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Daphnia Acute <u>48-hr EC50 (mg/L)</u>
C9 Olefin	4.62	0.41
C10 Alcohol	3.79	3.0

Test Substance:

68938-04-5 Nonene, HOF
68526-93-2 Nonene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an invertebrate 48-hour EC50 value of 0.41 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 3.0 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater invertebrates at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Reference:

Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Acute Alga Toxicity

Test Substance:	Other TS [CAS # 68938-04-5; 68526-93-2]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Algae (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS #'s 68938-04-5; 68526-93-2, which are complex, multi-constituent substances.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C9 Olefin	4.62
C10 Alcohol	3.79

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated alga acute toxicity values for 2 chemical components representative of the substances associated with CAS #'s 68938-04-5; 68526-93-2 are as follows:

Units/Value:

- Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Alga Acute <u>96-hr EC50 (mg/L)</u>
C9 Olefin	4.62	0.30
C10 Alcohol	3.79	2.0

Test Substance:

68938-04-5	Nonene, HOF
68526-93-2	Nonene, HOF, low-boiling

The two substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The two CAS numbers in this robust summary are listed on the TSCA inventory as UVCBs (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion: Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an alga 96-hour EC50 value of 0.30 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 2.0 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater green algae at levels more closely aligned with their olefinic components.

Reliability: (2) Reliable with restrictions

The toxicity values are calculated.

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Invertebrate Acute Toxicity

Test Substance:	Other TS [CAS # 68516-18-7]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Invertebrate (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS # 68516-18-7, which is a complex, multi-constituent substance.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C10 Olefin	5.12
C11 Alcohol	4.28

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results: Calculated invertebrate acute toxicity values for 2 chemical components representative of the substances associated with CAS # 68516-18-7 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Daphnia Acute <u>48-hr EC50 (mg/L)</u>
C10 Olefin	5.12	0.16
C11 Alcohol	4.28	1.2

Test Substance: 68516-18-7 Decene, HOF

The substance in this robust summary is in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The CAS number in this robust summary is listed on the TSCA inventory as UVCB (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion: Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an invertebrate 48-hour EC50 value of 0.16 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 1.2 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater invertebrates at levels more closely aligned with their olefinic components.

Reliability: (2) Reliable with restrictions

The toxicity values are calculated.

Reference: Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source): ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Acute Alga Toxicity

Test Substance:	Other TS [CAS # 68516-18-7]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Algae (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions:	Log Kow (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The Kow calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2).
<ul style="list-style-type: none">Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.	The following chemicals are representative of the substances associated with CAS # 68516-18-7, which is a complex, multi-constituent substance.

<u>Chemical</u>	Calculated <u>log K_{ow}</u>
C10 Olefin	5.12
C11 Alcohol	4.28

1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92.
2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Robust Summaries - Olefin Hydroformylation Products

Results:

Calculated alga acute toxicity values for 2 chemical components representative of the substances associated with CAS # 68516-18-7 are as follows:

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

<u>Chemical</u>	Calculated <u>log K_{ow}</u>	Alga Acute <u>96-hr EC50 (mg/L)</u>
C10 Olefin	5.12	0.12
C11 Alcohol	4.28	0.82

Test Substance:

68516-18-7 Decene, HOF

The substance in this robust summary is in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The CAS number in this robust summary is listed on the TSCA inventory as UVCB (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Based on the calculated Kow values, the olefinic fraction alone would be expected to exhibit an alga 96-hour EC50 value of 0.12 mg/L, while the alcohol fraction would be expected to exhibit an EC50 value of 0.82 mg/L. Based on chemical composition, the olefin hydroformylation products in this robust summary are expected to produce acute toxicity to freshwater green algae at levels more closely aligned with their olefinic components.

Reliability:

(2) Reliable with restrictions

The toxicity values are calculated.

Reference:

Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Robust Summaries - Olefin Hydroformylation Products

Calculated Water Solubility

Test Substance:	Other TS
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions:	Water Solubility estimations performed by WSKOWWIN are based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". <i>Environ. Toxicol. Chem.</i> 15 :100-106. 1995.
<ul style="list-style-type: none"> Note: Concentration prep., vessel type, replication, test conditions. 	

Results:

Units/Value:	<u>Alcohol Component</u>	<u>Calculated WS (mg/L)</u>	<u>Olefin Component</u>	<u>Calculated WS (mg/L)</u>
<ul style="list-style-type: none"> Note: Deviations from protocol or guideline, analytical method. 	C6	10,340-11,950	C5	210-245
	C7	3,539-11,950	C6	47-76
	C8	1,379-1,485	C7	16.9-33.8
	C9	164-614	C8	1.0-5.9
	C10	75.0*	C9	0.7-1.5
	C11	28.0*	C10	1.0
	C13	5.8*	C12	0.1

* Measured values (reported under a separate robust summary).

Test Substance:	68527-03-7	Pentene, HOF
	68938-02-3	Pentene, HOF, low-boiling
	70955-11-2	Hexene, HOF
	70955-03-2	Hexene, HOF, low-boiling
	68527-04-8	Heptene, HOF
	68526-96-5	Heptene, HOF, low-boiling
	68527-05-9	Octene, HOF
	68938-03-4	Octene, HOF, low-boiling
	68938-04-5	Nonene, HOF
	68526-93-2	Nonene, HOF, low-boiling
	68516-18-7	Decene, HOF
	68527-06-0	Dodecene, HOF
	68526-91-1	Dodecene, HOF, low-boiling
	68526-91-0	Dodecene, HOF, high-boiling

Robust Summaries - Olefin Hydroformylation Products

The substances in this robust summary are in the Olefin Hydroformylation Products Category. The substances in this category are composed of olefins and alkyl alcohols and are described as "alkyl alcohol bottoms". These substances are residual waste materials remaining from the production of alkyl alcohols. Hydroformylation refers to the reaction between a branched olefin and a mixture of carbon monoxide and hydrogen to produce an aldehyde, which is then hydrogenated to yield the alcohol. Low, intermediate, and high boiling alkyl alcohol bottom products are included in this category, each containing a mixture of hydroformylation reactants (olefins) and finished products (alcohols).

A specific composition for the substances in this category does not occur because the production process results in a variable composition.

The CAS numbers in this robust summary are listed on the TSCA inventory as UVCB (Unknown or Variable composition, Complex reaction products and Biological materials).

Conclusion:

Reliability:

(2) Reliable with restrictions

The results include values estimated using calculated K_{ow} values available in the WSKOWWIN program and represent a potential water solubility range for products with the CAS numbers listed under test substance.

Reference:

Meylan, M., SRC 1994-1999. WSKOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Other (source):

ExxonMobil Biomedical Sciences, Inc.

Olefin Hydroformylation Products Category
Robust Summaries
Mammalian Health Effects

CAS# 68527-03-7: Pentene, HOF
CAS# 68938-02-3: Pentene, HOF, low-boiling
CAS# 70955-11-2: Hexene, HOF
CAS# 70955-03-2: Hexene, HOF, low-boiling
CAS# 68526-80-7: Alcohols, C6 and C8 iso, distillation residues
CAS# 70955-04-3: Hexene, HOF, high-boiling
CAS# 68527-04-8: Heptene, HOF
CAS# 68526-96-5: Heptene, HOF, low-boiling
CAS# 68526-88-5: Heptene, HOF, high-boiling
CAS# 68527-05-9: Octene, HOF
CAS# 68938-03-4: Octene, HOF, low-boiling
CAS# 68526-89-6: Octene, HOF, high-boiling
CAS# 68938-04-5: Nonene, HOF
CAS# 68526-93-2: Nonene, HOF, low-boiling
CAS# 68526-90-9: Nonene, HOF, high-boiling
CAS# 68516-18-7: Decene, HOF
CAS# 68527-06-0: Dodecene, HOF
CAS# 68526-92-1: Dodecene, HOF, low-boiling
CAS# 68526-91-0: Dodecene, HOF, high-boiling

Revised by:
ExxonMobil Chemical Company
September 25, 2002

Robust Summaries - Olefin Hydroformylation Products

Olefin Hydroformylation Products and their corresponding constituents

CAS Number	Product name	Olefin	Alcohol
68527-03-7	Pentene, HOF	C5 (RA)	C6 (68526-79-4)
68938-02-3	Pentene, HOF, low-boiling	C5 (RA)	C6 (68526-79-4)
70955-11-2	Hexene, HOF	C6 (68526-52-3)	C7
70955-03-2	Hexene, HOF, low-boiling	C6 (68526-52-3)	C7 (70914-20-4)
68526-80-7	Alcohols, C6 and C8 iso, distillation residues	-	C6, C8 (68526-79-4) (111-27-3) (104-76-7)
70955-04-3	Hexene, HOF, high-boiling	-	C7-8 (68526-83-0) (104-76-7)
68527-04-8	Heptene, HOF	C7 (68526-53-4)	C8 (68526-83-0) (104-76-7)
68526-96-5	Heptene, HOF, low-boiling	C7 (68526-53-4)	C8 (68526-83-0) (104-76-7)
68526-88-5	Heptene, HOF, high-boiling	-	C8-9 (68526-83-0) (104-76-7)
68527-05-9	Octene, HOF	C8 (68526-54-5)	C9 (68526-84-1) (68515-81-1)
68938-03-4	Octene, HOF, low-boiling	C8 (68526-54-5)	C9 (68526-84-1) (68515-81-1)
68526-89-6	Octene, HOF, high-boiling	-	C9-10 (68526-84-1) (25339-17-7)
68938-04-5	Nonene, HOF	C9 (68526-55-6)	C10 (68526-85-2) (68526-84-1)
68526-93-2	Nonene, HOF, low-boiling	C9 (68526-55-6)	C10 (68526-85-2) (68526-84-1)
68526-90-9	Nonene, HOF, high-boiling	-	C10-11 (68526-85-2) (68526-84-1) (68526-86-3)
68516-18-7	Decene, HOF	C10 (RA)	C11 (85566-14-9) (68526-86-3)
68527-06-0	Dodecene, HOF	C12 (68526-58-9)	C13 (68526-86-3) (112-53-8)
68526-92-1	Dodecene, HOF, low-boiling	C10-12 (68526-58-9)	C13 (68526-86-3) (112-53-8)
68526-91-0	Dodecene, HOF, high-boiling	-	C13-14 (68526-86-3) (112-53-8)

Table of Contents

C6 Alcohol component: Hexanol, branched and linear (68526-79-4)

- Acute oral
- Acute dermal
- Acute inhalation
- Repeat dose - dermal
- Developmental toxicity (1-hexanol)

C6 Olefin component: Alkenes, C6 (68526-52-3)

- Mouse micronucleus (inhalation)
- Mouse micronucleus (oral)
- Ames assay

C7 Alcohol component: Alcohols, C6-8 branched (70914-20-4)

- Acute oral
- Acute dermal
- Acute inhalation

C7 Olefin component: Alkenes, C6-8, C7-rich (68526-53-4)

- Acute inhalation
- Acute dermal
- Mouse micronucleus (oral)

C8 Alcohol component: Alcohols, C7-9 branched (68526-83-0)

- Acute oral
- Acute dermal
- Acute inhalation
- Ames assay (2-ethyl-1-hexanol)
- Repeat dose (Iso-octanol)
- Repeat dose (dermal)
- Developmental toxicity (1-octanol)
- Developmental toxicity

C8 Olefin component: Alkenes, C7-9, C8 rich (68526-54-5)

- Acute oral
- Acute dermal
- Acute inhalation

C9 Alcohol component: Alcohols, C8-10 iso, C9 rich (68526-84-1)

- Acute oral
- Acute dermal
- Repeat dose (isononanol)
- Developmental toxicity (isononylalcohol 1)
- Developmental toxicity (isononylalcohol 2)

Developmental toxicity (1-nonanol)

C9 Hydroformylation Product (C₉HOF)

Acute oral

Acute dermal

C9 Olefin component: Alkenes, C8-10, C9 rich (68526-55-6)

Acute oral

Acute dermal

Acute inhalation

Mouse micronucleus

Ames assay

C10 Hydroformylation Product (C₁₀V-HOF)

Acute oral (C₁₀V-HOF)

Acute oral (C₁₀U-HOF)

Acute dermal (C₁₀V-HOF)

Acute dermal (C₁₀U-HOF)

C10 Alcohol component: Alcohols, C9-11 iso, C10 rich (68526-85-2)

Acute oral

Acute dermal

Developmental toxicity (isodecanol)

Developmental toxicity (1-decanol)

C7-9-11 Alcohol (85566-14-9)

Developmental toxicity

C13 Alcohol component: Alcohols, C11-14 iso, C13 rich

Acute oral

Ames assay (1-dodecanol)

Repeat dose toxicity

C12 Olefin component: Alkenes, C11-13, C12 rich (68526-58-9)

Acute oral

Acute dermal

Acute inhalation

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Hexanol, branched and linear 68526-79-4
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment	Other Oral LD ₅₀ Pre-GLP 1960 Rats/Sprague-Dawley Males 5 rats/dose Gastric Intubation None Single exposure 26, 82, 259, 820, 2591, 8200 mg/kg None
Remarks on Test Conditions	After a three to four hour fasting period, groups of 5 rats received the test material at dose levels of 26, 82, 259, 820, 2591, and 8200 mg/kg of body weight. The results were converted to weight units by means of the specific gravity. Observations for signs of toxicity were made immediately and at one and 24 hours after compound administration and daily for a period of 7 days. Gross necropsy examinations were performed on all animals that died or were killed.
Results	LD ₅₀ = 3670 mg/kg
Remarks	None of the animals died in the 26, 82, 259, and 820 mg/kg dose groups. One of the animals in the 2591 mg/kg group died within 24 hours of dosing. All animals in the 8200 mg/kg group died within 4 hours following dose administration. Treatment resulted in depression (i.e. inactivity, depressed righting reflexes, ataxia) and labored respiration. These signs had an early onset and recovery was complete by the second day after dosing. Gross necropsy on the animals that died showed congested kidneys. Also, animals that died during the first hour after administration showed evidence of gastrointestinal irritation.
Conclusions	Under the conditions of this study, Hexanol, branched and linear has a low order of acute oral toxicity in rats.
Data Quality	1 - Valid without restrictions
Reference	Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report.
Date last changed	September, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Hexanol, branched and linear 68526-79-4
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment	Other Acute dermal toxicity Pre-GLP 1960 Albino Rabbits Males and Females 2 rabbits/sex/dose Dermal Application None Single exposure 82, 259, 820, and 2600 mg/kg None
Remarks on Test Conditions	A single dermal application of the test material was made to four groups of four rabbits at doses of 82, 259, 820, and 2600 mg/kg. The results were converted to weight units by means of the specific gravity. The test material was applied to intact abdominal skin and covered with an occlusive covering for 24 hours. Observations for signs of toxicity were made at one, four and 24 hours after compound administration and thereafter for a total of 7 days. Gross necropsies were performed on all animals at the end of the observation period.
Results	LD ₅₀ > 2600 mg/kg
Remarks	There were no mortalities at any dosage level tested. The LD ₅₀ in albino rabbits is greater than the highest dose tested (approx. 2.6 g/kg body weight). Signs of toxicity included labored respiration and central nervous system depression. All animals recovered within 4-48 hours after the exposure period began. Moderate erythema and edema were observed.
Conclusions	Under conditions of this study, Hexanol, branched and linear has a low order of acute dermal toxicity in rabbits.
Data Quality	2 - Valid with restrictions.
Reference	Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report.
Date last changed	September, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Hexanol, branched and linear 68526-79-4
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment	Other Inhalation LC ₅₀ Pre-GLP 1960 Rats/Wistar, Mice/Swiss, Guinea Pigs/English short hair Males 10/species Inhalation NA Single 6 hour exposure 1060 ppm None
Remarks on Test Conditions	Rats, mice, and guinea pigs received a single, 6-hour exposure to the test material in air. Exposures were at atmospheres nearly saturated with vapors of the alcohol (1060 ppm). The exposure was conducted in a 500-liter stainless steel inhalation chamber equipped at the inlet with a device for generating a near-saturated vapor of the test material. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml. of the test material. Air flow through each bubbler was 18 liters/minute, so the total flow through the chamber was 36 liters/min. Actual chamber concentration was not measured during the exposure. The theoretical chamber concentration was calculated to be 1060 ppm based upon the amount of test material that vaporized and the rate of air flow. During exposure, all animals were observed for gross signs of toxicity at 30-minute intervals. Gross necropsies were performed on animals 24 hours after exposure.
Results	LC ₅₀ > 1060 ppm for rats, mice and guinea pigs.
Remarks	No deaths were seen during or after the exposure period. Thirty minutes after exposure, slow, deep respiration was observed in all three species. After 90 minutes of exposure, all three species exhibited gasping, labored respiration, lacrimation and nasal discharge. These signs persisted until the termination of exposure. Gross necropsy results indicate that the test material produced slight lung congestion in all animals. All other tissues and organs were unremarkable.
Conclusions	Under the conditions of this study, Hexanol, branched and linear has a low order of acute inhalation toxicity in rats, mice and guinea pigs.
Data Quality	2 - Valid with restrictions - No analysis of exposure atmosphere.
Reference	Hazleton Laboratories (1960). Acute oral administration, acute dermal application, and acute inhalation exposure. Unpublished report.
Date last changed	September, 2000

Robust Summaries - Olefin Hydroformylation Products

Repeat Dose Toxicity

Test Substance CAS No.	Hexanol, branched and linear 68526-79-4
Method/Guideline	Other
Test Type	Repeated Dermal Application
GLP	Pre-GLP
Year	1961
Species/strain	Albino Rabbits
Route of administration	Dermal
Duration of test	12 days
Number of animals	8 (2/sex/dose)
Dose/Conc. Levels	0.4 g/kg and 2.0 g/kg
Sex	Males and Females
Frequency of treatment	Single daily treatment for 10 days
Control group and treatment	Isopropyl alcohol
Remarks on Test Conditions	<p>Undiluted control and test materials were applied to intact skin of the animals. Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each application and at study termination.</p> <p>Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application and brain, liver, kidney, and blood samples were taken. In addition, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved.</p>
<u>Results</u>	NOAEL for systemic toxicity = 2.0 g/kg
Remarks	There was no evidence of systemic toxicity at either dose of the test substance. Histopathological findings were unremarkable. Repeated application of the test material to the skin of albino rabbits at both dose levels produced moderate to marked degree of irritation. A slight to marked degree of edema was observed in two low-dose animals and three high-dose animals following one or more of the first three applications. Also, the exposed skin of two high-dose animals showed necrosis.
Conclusions	Under the conditions of this study, Hexanol, branched and linear can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study.
Data Quality	2 - Valid with restrictions.
Reference:	Esso Research and Engineering Company (1961). Unpublished Report.
Date last changed	September, 2000

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Robust Summaries - Olefin Hydroformylation Products

Conclusions	Inhalation of saturated vapors of 1-hexanol is not maternally toxic or teratogenic in rats.
Data Quality	2 - Reliable with restrictions.
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology evaluation of 1-pentanol, 1-hexanol, and 2-ethyl-1-hexanol administered by inhalation to rats." (1989) <u>Journal of the American College of Toxicology</u> 8(2) : 405-410. NIOSH, Division of Biomedical and Behavioral Sciences
Date last changed	13-Sep-00

Robust Summaries - Olefin Hydroformylation Products

Genetic Toxicity

Test Substance CAS No.	Alkenes, C6 68526-52-3
Method Type of Study	EPA OTS 798.5395 Mouse Micronucleus
GLP Year Species/Strain	Yes 1993 Mouse/ B6C3F1
Sex Number/sex/dose Route of administration Vehicle Exposure Period Concentrations	Male and Female 15/sex Inhalation NA 6 hours/day for 2 consecutive days Target exposure: 1000 ppm; Actual mean exposure: 1057 ppm (Saturated vapors, no aerosol)
Controls	Positive: Cyclophosphamide (40 mg/kg) in water by oral gavage Negative: Air (Sham exposure)
Statistical Methods	To determine the percentage of micronuclei, 1000 polychromatic erythrocytes from each animal were examined for micronuclei. To determine the percentage of polychromatic erythrocytes, the number of polychromatic erythrocytes in a total of 1000 erythrocytes was determined. Statistical analysis included calculation of means and standard deviations of the micronuclei data and a test of equality of group means by a standard one way analysis of variance at each time period. When the ANOVA was significant, comparisons of carrier control to dosed group means were made according to Duncan's Multiple Range Test. Data from both males and females were analyzed as a single group to facilitate comparisons to published data.
Remarks on Test Conditions	Vapors were generated by delivering the test material with a piston pump to a glass cylinder with heating tape. Vapors were drawn into the chamber with air flow at a rate of 200 liters/minute. Nominal and actual concentrations were determined by net weight loss of the test material and by gas chromatography, respectively. Animals were exposed to vapors of the test substance for 6 hours per day on 2 consecutive days. During each exposure, animals were observed hourly. The positive control, cyclophosphamide, was administered by oral gavage as a single dose. Animals from the treated group were sacrificed by carbon dioxide asphyxiation at appropriately 24 hours after the second day of exposure. Animals treated with cyclophosphamide were sacrificed 24 hours following dose administration. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange.
<u>Results</u>	Negative
Remarks for Results	The test material was not clastogenic since it did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, indicating that the test substance is not clastogenic. In addition, the test substance did not induce a statistically significant decrease in the mean percent of polychromatic erythrocytes, indicating that the test substance did not induce bone marrow toxicity. The positive control did induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes and was therefore clastogenic. The sham control values for the mean number of micronucleated polychromatic erythrocytes were within the normal range for the negative control.

Robust Summaries - Olefin Hydroformylation Products

Conclusions	Under the conditions of this assay, Alkenes, C6 are not clastogenic following inhalation exposure in mice.
Data Quality	1 - Reliable without restrictions
Reference	"In vivo mammalian bone marrow micronucleus assay: inhalation dosing method," Exxon Biomedical Sciences, Inc. 1991
Date last changed	December, 2000

Genetic Toxicity

Test Substance CAS No.	Alkenes, C6 68526-52-3
Method Type of Study	EPA OTS 798.5395 Mouse Micronucleus
GLP Year Species/Strain	Yes 1991 Mouse/ B6C3F1
Sex Number/sex/dose Route of administration Vehicle Exposure Period Concentrations	Male and Female 15/sex Oral gavage NA Single dose 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study.
Controls	Positive: Cyclophosphamide (40 mg/kg) Negative: Corn oil
Statistical Methods	To determine the percentage of micronuclei, 1000 polychromatic erythrocytes from each animal were examined for micronuclei. To determine the percentage of polychromatic erythrocytes, the number of polychromatic erythrocytes in a total of 1000 erythrocytes was determined. Statistical analysis included calculation of means and standard deviations of the micronuclei data and a test of equality of group means by a standard one way analysis of variance at each time period. When the ANOVA was significant, comparisons of carrier control to dosed group means were made according to Duncan's Multiple Range Test. A standard regression analysis was performed to test for a dose response. Sexes were analyzed separately.
Remarks on Test Conditions	The test material and the carrier were administered by oral gavage as a single dose to mice (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose. Animals from the appropriate groups were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange.
<u>Results</u>	Positive

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Remarks for Results	<p>The test material induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes per 1000 cells at 5.0 g/kg for the 24-hour males and females (6.8 +/- 3.12 and 5.4 +/- 2.1, respectively). The mean number of micronucleated polychromatic erythrocytes for the positive controls at 24 hours for males and females were 36.2 +/- 10.5 and 30.4 +/- 9.0 and the negative controls were 2.4 +/- 0.9 and 2.6 +/- 1.5. The increase in micronucleated polychromatic erythrocytes observed at 24 hours was dose-related. However, at 48 and 72 hours after the initial exposure, the mean number of micronuclei did not differ between the control and treated groups. The test substance did not induce a statistically significant decrease in the mean percent of polychromatic erythrocytes, indicating that the test substance is not toxic to bone marrow. The positive control induced significant increases in the mean number of micronucleated polychromatic erythrocytes. The positive control also induced a statistically significant decrease in the mean percent of micronucleated polychromatic erythrocytes in male mice. Carrier control values for the mean percent of micronucleated polychromatic erythrocytes and the mean number of micronucleated polychromatic erythrocytes were within the normal range for the negative controls.</p> <p>Alkenes, C6 produced a slight, transient increase in micronucleated polychromatic erythrocytes at the highest level by oral gavage. However, given that inhalation is the primary route of industrial exposure, a micronucleus study was repeated with inhalation as the route of administration. This study produced negative results (IUCLED section 5.6). In addition, Alkenes, C6 are not mutagenic <i>in vitro</i>. Collectively, these data suggest that Alkenes, C6 are not expected to be genotoxic.</p>
Conclusions	<p>Under the conditions of this study, Alkenes, C6 were clastogenic to the bone marrow of B6C3F1 mice when administered by oral gavage at 5.0 g/kg 24 hours prior to analysis, but not at 48 and 72 hours post-exposure.</p>
Data Quality	<p>1 - Reliable without restrictions</p>
Reference	<p>"In vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Method," Exxon Biomedical Sciences, Inc., 1991.</p>
Date last changed	<p>December, 2000</p>

Genetic Toxicity

Test Substance CAS No.	Alkenes, C6 68526-52-3
Method/Guideline Test Type GLP Year	EPA OTS 798.5265 Bacterial Mutagenicity - Ames Assay Yes 1991
Species/strain	Salmonella typhimurium; TA98; TA100; TA1535; TA1537; TA1538
Metabolic Activation	With and without S9 fraction of livers from rats pretreated with Aroclor 1254.
Dose/Conc. Levels	3.2, 10, 32, 100 and 320 µg/plate (Doses were based on a pre-test for toxicity)
Statistical methods	The mean plate count and standard deviation for each dose point were determined. Any test value that was equal to or greater than three times the mean value of the concurrent vehicle control was considered to be a positive dose.
Remarks on Test Conditions	
Solvent:	DMSO was used for controls; Ethanol was used for the test material
Positive Controls:	2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine
Negative Controls:	Vehicle controls were dosed at 0.1 ml/plate ethanol and 0.1 ml/plate DMSO
	To determine the highest dose of compound to be used in the assay, a dose range from 1 to 10,000 µg/plate was tested. Only strain TA98 was used. The toxicity pretest was repeated and toxicity was observed as a reduction in both background and revertant colony counts. 320 µg/plate was selected as the high dose to be used on the mutagenesis assay for both the saline (-S9) and the +S9 treated plates.
	A repeat assay was performed in order to verify the data produced in the initial assay.
Results	Negative
Remarks	The test material did not induce a dose related increase in the mutation frequencies of any of the tester strains either in the presence or absence of metabolic activation. All positive and negative controls responded in a manner consistent with data from previous assays.
Conclusions	Under the conditions of this study the test material is not mutagenic for the Salmonella tester strains at doses up to and including 320 µg/plate.
Data Quality	1 - Valid without restrictions
Reference:	Microbial Mutagenesis in <i>Salmonella</i> : Mammalian Microsome Plate Incorporation Assay; Exxon Biomedical Sciences, Inc., 1991.
Date last changed	December, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Alcohols, C6-8 branched 70914-20-4
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment	Other Acute oral toxicity Not specified 1979 Rats/Sprague/Dawley Males 5/dose Oral Intubation None Single Exposure 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg None
Remarks on Test Conditions	Animals were fasted for approximately 18 hours prior to dosing. The undiluted test material was administered by oral intubation at doses of 1.0, 1.47, 2.15, 3.16, 4.64, 6.81 and 10.0 g/kg (5 rats/dose). Animals were observed for signs of toxicity at 1, 2, and 4 hours after dosing and daily thereafter for fourteen days.
Results	LD ₅₀ = 3.9 g/kg
Remarks	All animals in the 6.81 and 10.00 g/kg groups died. Two of the five animals in the 4.64 g/kg group died and 1 animal each in the 1.00, 2.15, and 3.15 g/kg groups died. No animals in the 1.47 g/kg group died. Except for one animal in the 2.15 g/kg group, all animals that died did so within three days of dosing. Signs of toxicity observed included respiratory rate decreases, fecal staining, decreased motor activity and hypothermia.
Conclusions	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute oral toxicity.
Data Quality	2 - Valid with restrictions - only one sex tested.
Reference	"Acute Oral Toxicity Study in Rats," Esso Research and Engineering (1979). Unpublished report.
Date last changed	September, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels Control group and Treatment	Alcohols, C6-8 branched 70914-20-4 Other Acute dermal toxicity Not specified 1979 Albino Rabbits/New Zealand White Males and Females 2 rabbits/sex/dose Dermal None Single dose 50, 200, 794 and 3,160 mg/kg None
Remarks on Test Conditions	Doses of 50, 200, 794 and 3160 mg/kg were administered to sixteen rabbits (two/sex/dose level). The undiluted test material was applied to intact skin and the animal was then wrapped in an impervious plastic sleeve. Following approximately 24 hours of exposure, the wrappings were removed and the test site was wiped free of excess test material. After 30 minutes, dermal observations were made. Observations were recorded at 1, 2 and 4 hours after dosing and daily thereafter for 14 days.
Results	LD ₅₀ > 3,160 mg/kg of body weight.
Remarks	There were no deaths at any dose level in either sex. All animals at the 50 mg/kg level exhibited very slight erythema and no edema. Well-defined erythema without edema was observed in animals at 200 and 794 mg/kg dose levels. At the 3160 mg/kg dose level one animal exhibited moderate to severe erythema and three animals exhibited areas of necrosis. Necropsy examinations did not reveal any significant abnormalities. Dark red foci were observed in the lungs of males (50mg/kg) and females (3,160 mg/kg), however this effect was not dose-related. Dark red foci of the adrenals were observed in males and females at 200, 794, and 3,160 mg/kg.
Conclusions	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute dermal toxicity in rats.
Data Quality	2 - Valid with restrictions - GLP not specified.
Reference	Esso Research and Engineering (1979). Unpublished report.
Date last changed	September, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Alcohols, C6-8 branched 70914-20-4
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels	Other Acute inhalation toxicity Not specified 1979 Rats/Sprague-Dawley, Mice/Swiss albino, Guinea pigs/Hartley Males and Females 5/sex/dose Inhalation NA Single, 6 hour exposure 0, 152 ppm
Remarks on Test Conditions	Animals (5/sex/dose) were held for a minimum equilibration period of 12 days. Animals were exposed to 152 ppm of the test material for six hours. To generate vapors, room air was drawn through the test material at a flow rate of 103 l/min. The resulting maximum attainable vapors were passed through a Kjeldahl trap and flask prior to entering the glass exposure chamber containing the test animals. Weight loss was determined following exposure and was taken to be equal to the amount of test material delivered during exposure. The weight loss was divided by the total volume of air passed through the chamber to give the nominal concentration. All three species were exposed in the same chamber. For each species, a control group was also sham-exposed to room air. The animals were observed for abnormalities prior to exposure, at 15-minute intervals during the first hour of exposure and then hourly for the remainder of exposure. Subsequent evaluations were made for a total of 14 days. After fourteen days, gross necropsy was performed.
Results	LC ₅₀ > 152 ppm
Remarks	No abnormalities were noted in the control or exposed rats, mice or guinea pigs during the exposure period. Upon removal from the chamber, dry rales (1/10) and excessive salivation (2/10) were observed in exposed rats. During the 14-day observation period, excessive salivation was observed in mice (4/10) and nasal discharge (2/10) occurred. Necropsy examination revealed an increased incidence of lung discoloration in treated rats (6/10) and guinea pigs (8/10).
Conclusions	Under the conditions of this study, Alcohols, C6-8 branched have a low order of acute inhalation toxicity in rats.
Data Quality	2 - Valid with restrictions - Vapor concentration not analyzed.
Reference	Esso Research and Engineering (1980). Unpublished Report.
Date last changed	September, 2000

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:	Alkenes, C6-8, C7 rich 68526-53-4 NA Inhalation LC ₅₀ Pre-GLP 1979 Swiss albino Mice, Sprague-Dawley Rats, Hartley Guinea Pigs Males and Females 5/sex/species Inhalation NA Single Dose 42.3 mg/L for 6 hours; vapors only Control animals (5/sex/species) were exposed to clean air as a sham exposure.
Remarks on Test Conditions	<p>Room air, at a flow rate of 134 l/minute was bubbled through test material in a flask to produce a vapor-laden airstream that was directed, undiluted, into the exposure chamber. The nominal exposure concentration was calculated by dividing the mass of test material consumed by the total volume of air passing through the chamber.</p> <p>Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Body weights were recorded on Days 0, 1, 2, 4, 7, and 14. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. During the necropsies, the lungs with trachea, kidneys, and liver were preserved for possible histopathological examination.</p>
Results (LD₅₀ or LC₅₀):	LC₅₀ > 42.3 mg/L for 6 hours
Remarks	<p>In mice, exposure to 42.3 mg/L of the test substance resulted in 1 death 1 hour into the exposure period. All other mice survived until the end of the study. None of the rats died during the study. Two guinea pigs died by 45 minutes into the exposure period. The remaining guinea pigs survived until the end of the study. All exposed species exhibited signs of systemic toxicity including labored breathing, prostration, body tremors, and ataxia during the exposure. However, in the surviving animals, these signs completely reversed within 24 hours following the exposure. Liver discoloration was noted upon necropsy in the mouse and the two guinea pigs that died during the exposure. Otherwise, no significant findings were observed at necropsy.</p>
Conclusions	<p>Under conditions of this study, Alkenes, C6-8, C7 rich have a low order of acute inhalation toxicity in rodents.</p>
Data Quality	2 - Valid with restrictions - no analysis of exposure atmosphere.
Reference	<p>"An Acute Inhalation Toxicity Study of MRD-ECH-78-32 in the Mouse, Rat, and Guinea Pig," Bio/dynamics, Inc. for Exxon Research and Engineering Company, May 25, 1979.</p>
Date last changed	October, 2000

Acute Toxicity

Test Substance CAS No.	Alkenes, C6-8, C7 rich 68526-53-4
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:	NA Dermal LD ₅₀ Pre-GLP 1978 Albino rabbits Males and Females 2/sex/dose Dermal NA Single 24-hour exposure 200 and 3160 mg/kg. NA
Remarks on Test Conditions	Undiluted test material was applied to clipped, abraded abdominal skin under gauze and thick plastic. Following the 24-hour exposure period, the wrapping was removed and the exposed area was wiped to remove residue. Animals were observed for gross signs of irritation and systemic toxicity 1,2,3, and 4 hours post dose and daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually.
Results (LD₅₀ or LC₅₀):	LD₅₀ > 3160 mg/kg
Remarks	No mortalities were observed at any dose tested. Lethargy and ataxia were observed in all animals, but these symptoms cleared by Day 2. Dermal reactions were generally moderate at 200 mg/kg and cleared by Day 14. In the high dose group, more severe dermal reactions, including moderate edema and severe erythema, persisted through the study. No significant fluctuations in body weight occurred. Necropsy findings were unremarkable except for a pus-filled liver in 1 rabbit from the high dose group.
Conclusions	Alkenes, C6-8, C7 rich have a low order of acute dermal toxicity.
Data Quality	1 - Reliable without restrictions
Reference	MB Research Laboratories, Inc., Acute Dermal Toxicity in Albino Rabbits, 1978.
Date last changed	October, 2000

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Genetic Toxicity

Test Substance CAS No.	Alkenes, C6-8, C7 rich 68526-53-4
Method Type of Study GLP Year Species/Strain	EPA OTS 798.5395 Mouse Micronucleus Yes 1993 Mouse/ B6C3F1
Sex Number/sex/dose Route of administration Vehicle Exposure Period Concentrations	Males and Females 15/sex Oral gavage NA Single dose 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study.
Controls	Positive: Cyclophosphamide (40 mg/kg) Negative: Corn oil
Statistical Methods	Analysis of variance (ANOVA), Duncan's Multiple Range Test
Remarks on Test Conditions	The test material and the carrier were administered by oral gavage as a single dose to mice (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose. Animals from the appropriate groups were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange.
<u>Results</u>	Negative
Remarks for Results	There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, indicating that the test material was not clastogenic. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, which indicates that the positive control is clastogenic. The test material did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. In addition, the test material did not induce a significant decrease in the mean percent of polychromatic erythrocytes, which is a measure of bone marrow toxicity.
Conclusions	Under the conditions of this study, the test sample is not considered to be mutagenic at doses up to and including 5.0 g/kg.
Data Quality	1 - Reliable without restrictions
Reference	Exxon Chemical Company (1993). In Vivo Mammalian Bone Marrow Micronucleus Assay: Oral Gavage Dosing Method. Unpublished Report..
Date last changed	October, 2000

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Acute Toxicity

Test Substance CAS No.	Alcohols, C7-9 branched 68526-83-0
Method/Guideline	OECD 401
Type of Study	Acute oral toxicity
GLP	Yes
Year	1988
Species/strain	Rats/Wistar
Sex	Males and Females
No. of animals/sex/dose	5/sex/dose
Route of administration	Oral gavage
Vehicle	None
Frequency of Treatment:	Single Dose
Dose/Concentration Levels	2000 mg/kg
Remarks on Test Conditions	After being fasted for 12 to 18 hours, animals were administered a single oral gavage dose of 2,000 mg/kg of the undiluted test article. Observations were made four times on day 1; and daily for 14 days.
Results	LD ₅₀ > 2000 mg/kg
Remarks	Following dosing, the following symptoms were observed: sedation, ventral body position in males, hunched posture, and ruffled fur. However, all animals had recovered within 6 days of dosing. At necropsy, no macroscopic abnormalities were observed.
Conclusions	Under the conditions of this study, Alcohols, C7-9 branched has a low order of toxicity.
Data Quality	1 – Reliable without restrictions
Reference	“Acute oral toxicity study with Alcohols, C7-9 branched in rats,” (1988) unpublished report (RCC Research and Consulting Co. AG).
Date last changed	September, 2000

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Acute Toxicity

Test Substance CAS No.	Alcohols, C7-9 branched 68526-83-0
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of treatment Dose/Concentration Levels Control group and treatment	Other Acute dermal toxicity Pre-GLP 1960 Albino Rabbits Males and Females 4 rabbits/sex/dose Dermal; with occlusive binding Single 24 hour exposure 83, 262, 820, 2623 mg/kg (undiluted) None
Remarks on Test Conditions	The test substance was applied dermally to rabbits (4/sex/dose) under occlusive binding and removed after 24 hours. The results were converted to weight units by means of the specific gravity. Animals were observed 1, 4, and 24 hours after initial application of Alcohols, C7-9 branched and once daily for the next 7 days. At the termination of the study, survivors were weighed and gross necropsies were performed.
Results	Dermal LD ₅₀ > 2623 mg/kg
Remarks	Animals in the 83, 262, and 820 mg/kg dose groups exhibited normal appearance and behavior throughout the study. At the highest dose (2623 mg/kg), animals exhibited labored respiration and were inactive. One animal in the high dose group died within 24 hours. The remaining animals in this dose group returned to normal appearance and behavior 2 days after the treatment.
Conclusions	Alcohols, C7-9 branched showed a low order of acute dermal toxicity under the conditions of this study.
Data Quality	1 - Reliable without restrictions
Reference	Hazleton Labs (1960). Acute oral, acute dermal, and acute inhalation toxicity. Unpublished report.
Date last changed	September, 2000

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Acute Toxicity

Test Substance CAS No.	Alcohols, C7-9 branched 68526-83-0
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels	Other Acute inhalation toxicity Pre-GLP 1960 Rats/Wistar, Mice/Swiss, Guinea pigs/English Short Hair Males 10/species Inhalation NA Single 6 hour exposure Saturated Vapors
Remarks on Test Conditions	Rats, mice, and guinea pigs were exposed to near-saturation levels (200 ppm) of vapors of Alcohols, C7-9 branched in a 500 L stainless steel inhalation chamber for 6 hours. Vapor was generated by using two separate fritted disk glass bubblers, connected in parallel, each containing 200 ml of the test substance. Air flow through each bubbler was 18 l/m, and the total flow through the chamber was 36 l/m. Actual chamber concentration was not measured; theoretical chamber concentration was calculated to be 200 ppm. Animals were observed at one-hour intervals during the exposure. Animals were observed 24 hours following exposure and then necropsies were performed.
Results	LC ₅₀ > 200 ppm
Remarks	There were no deaths during the treatment period. There were no apparent signs of toxicity or alterations to behavior other than blinking in rats and mice. No macroscopic abnormalities were observed at necropsy.
Conclusions	Under the conditions of this study, Alcohols, C7-9 branched has a low order of acute inhalation toxicity in rats, mice and guinea pigs.
Data Quality	2 - Valid with restrictions. No analysis of exposure atmosphere.
Reference	Hazleton Labs (1960). Acute oral, acute dermal, and acute inhalation toxicity. Unpublished report.
Date last changed	September, 2000

Genetic Toxicity

Test Substance CAS No.	2-Ethyl-1-hexanol 104-76-7
Method	Other
Type of Study	Ames Assay
Test System	<i>S. typhimurium</i> , <i>E. coli</i>
GLP	Not specified
Year	1985
Species/Strain	<i>Salmonella typhimurium</i> /TA98; TA100; TA1535; TA1537; TA1538; <i>E. coli</i> WP2uvrA
Metabolic Activation	S9 mixture
Concentrations	1, 5, 10, 50, 100, 500, and 1000 ug/plate.
Statistical methods	Samples were run in duplicate. No further details provided.
Remarks on Test Conditions	2-Ethyl-1-hexanol (98% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (Polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)-acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls.
<u>Results</u>	Negative
Remarks for Results	In all of the strains tested, there was no evidence of mutagenicity of 2-ethyl-1-hexanol in the presence or absence of metabolic activation. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 2-ethyl-1-hexanol samples.
Conclusions	2-Ethyl-1-hexanol is not mutagenic in bacteria under the conditions of this study.
Data Quality	2- Reliable with restrictions (Similar to OECD 471)
Reference	H. Shimizu, Y. Suzuki, N. Takemura, S. Goto, H. Matsushita, (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," <i>Japanese Journal of Industrial Health</i> , 27: 400-419.
Date last changed	October 3, 2000

Repeat Dose Toxicity

Test Substance	Iso-octanol
CAS No.	--
Method/Guideline	NA
Type of Study	14-day repeat dose
GLP	Not specified
Year	1984
Species/strain	Rats/Wistar
Sex	Male
No. of animals/sex/dose	5/treatment, 10/control; 1mmol/kg/day of iso-octanol (130 mg/kg/day)
Route of administration	Oral gavage.
Duration of test	14 days
Frequency of treatment	Once daily for 14 days
Vehicle	Polyethylene glycol 300
Statistics	Mean values compared to controls by Student's t-test.
Remarks on Test Conditions	After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined.
Results	NOAEL = 130 mg/kg/day
Remarks	Iso-octanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Iso-octanol did not induce any changes in glycogen vacuolation or fat vacuolation. The activity of peroxisome-associated enzymes and levels of cholesterol and triglyceride were not significantly different between animals treated with iso-octanol and vehicle controls. No hyperlipidemia was observed.
Conclusions	Under the conditions of this study, iso-octanol had a low order of sub-acute toxicity in male rats for the endpoints studied.
Data Quality	2 - Reliable with restrictions - Not a guideline study.
Reference	C. Rhodes, T. Soames, M.D. Stonard, M.G. Simpson, A.J. Vernall, C.R. Elcombe, "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," (1984). <u>Toxicology Letters</u> 21: 103-109.
Date last changed	13-Sep-00

Repeat Dose Toxicity

Test Substance CAS No.	Alcohols, C7-9 branched 68526-83-0
Method/Guideline	Other
Test Type	Repeated Dermal Application
GLP	Pre-GLP
Year	1961
Species/strain	Albino Rabbits
Route of administration	Dermal
Duration of test	12 days
Number of animals	8 rabbits (2/sex/dose)
Dose/Conc. Levels	0.4 g/kg and 2.0 g/kg
Sex	Males and Females
Frequency of treatment	Single Daily treatment for 10 days
Control group	Isopropyl alcohol, 2/sex
Statistical methods	Not specified
Remarks on Test Conditions	Undiluted control and test materials were applied to intact skin of the animals (2/sex/dose). Materials were applied once daily for a total of ten applications with a one-day rest period between the third and fourth and eighth and ninth applications. The exposed skin area of each animal was approximately 10% of the total body surface at the 0.4 g/kg dosage level and approximately 40% of the total body surface at the 2.0 g/kg dosage level. After the first application, exposed skin was covered by rubber dental damming. In subsequent applications, loose gauze and adhesive tape were used to cover the exposed area since the authors felt that the damming itself may have induced some irritation. Each exposure period lasted approximately 18-24 hours. Animals were observed daily throughout the study and body weights were recorded prior to each exposure and at study termination. Clinical hematology and urinalysis were performed at the beginning of the study and 24 hours after the final application of test material. Animals were sacrificed 48 hours after the tenth application, samples of brain, thyroid, lung, heart, liver, kidneys, adrenals, skin, and bone marrow were preserved.
<u>Results</u>	NOAEL for systemic toxicity = 2.0 g/kg
Remarks	Animals in all exposure groups displayed normal appearance and behavior throughout the study. Although a slight decrease in body weight was observed initially, animals regained weight by the end of the study. Repeat application of the control substance, isopropyl alcohol produced slight irritation characterized by slight to moderate erythema, atonia, and desquamation. Repeated application of Alcohols, C7-9 branched resulted in moderate to severe irritation. Fissuring and coriaceous skin were also observed at both the low and high dose levels. Necrosis was observed in the high dose animals as well. Clinical studies did not indicate any other signs of toxicity. There was a general increase in the hematocrit and erythrocyte values at the end of the study.

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Conclusions	Under the conditions of this study, Alcohols, C7-9 branched can produce moderate skin irritation following repeated dermal exposures. However, the test material did not produce any evidence of systemic toxicity under the conditions of this study.
Data Quality	2 - Valid with restrictions
Reference	Esso Research and Engineering Company (1961). Repeat Dermal Application of Alcohols, C7-9 branched, Unpublished Report.
Date last changed	September, 2000

Developmental Toxicity

Test Substance CAS No.	1-Octanol NR
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of treatment Dose/Concentration Levels Control group and treatment Statistical methods	Other Developmental Toxicity Not specified 1989 Rats/Sprague-Dawley Pregnant females 15/dose Inhalation 7 hrs/day; Gestation days 1-19 400 mg/m ³ 15 sham-exposed rats MANOVA, ANOVA, Kruskal-Wallis test
Remarks on Test Conditions	Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was $\geq 99\%$ as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 400 mg/m ³ . Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO ₂ asphyxiation, and the uterus and ovaries were removed and examined for corpora lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.
Results	Maternal and Developmental NOAEL ≥ 400 mg/m ³

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Remarks	No treatment-related effects were observed in dams. There were no significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups.
Conclusions	Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Octanol does not induce maternal or fetal toxicity.
Data Quality	2 - Reliable with restrictions
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) <u>Journal of the American College of Toxicology</u> 9(1): 93-97. NIOSH, Division of Biomedical and Behavioral Sciences.
Date last changed	February, 2001

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Developmental Toxicity

Test Substance CAS No.	Alcohols, C7-9 branched 68526-83-0
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/dose Route of administration Exposure period Dose/Concentration Levels Control group and treatment Statistical methods	OECD 414 Developmental Toxicity Yes 1994 Rat/Sprague-Dawley Females 25/dose Oral gavage GD 6-15 100, 500, and 1000 mg/kg/day Carrier only - corn oil Nested analysis of covariance, Least Significant Difference (LSD), Chi-square, Fisher Exact test, Armitage's test.
Remarks on Test Conditions	Mated females were assigned to dose groups of 100, 500, and 1000 mg/kg/day or to a corn oil-only group (25/dose). The test substance was administered in volumes of 5 ml/kg. Body weight and food consumption measurements were made on GD 0, 6, 9, 12, 15, 18, and 21. The animals were examined for viability twice daily during the treatment period and once daily thereafter. Clinical observations were made daily during gestation. On GD 21, animals were sacrificed and cesarean sections and necropsies were performed. Uterine weights with ovaries attached were recorded, uterine contents were examined, and implantation data were recorded. All live fetuses were weighed, sexed externally, and examined externally for gross malformations. Approximately one-half of the fetuses were prepared for examination of abnormalities in the head and the other half were preserved for examination of skeletal abnormalities.
Results	Maternal NOAEL = 500 mg/kg/day Fetal NOAEL = 1000 mg/kg/day
Remarks	One animal in the high dose group was euthanized in moribund condition on GD 9. The animal had extreme abdominal staining just prior to death, but there were no significant findings at postmortem examination and the cause of morbidity was therefore not established. Adverse clinical signs were observed in 8 of the 24 dams in the high dose group. These signs included emaciation, decreased food consumption, abdominal/anogenital staining, rales, hypoactivity, and little or no stool. The symptoms were transient and generally were not observed following cessation of dosing. The remaining dams in the high dose group had incidental findings such as alopecia, but otherwise appeared normal throughout the study. There were no observable abnormalities in dams of the middle and low dose groups throughout the gestational period. In the high dose group, statistically significant decreased body weight gain and food consumption were observed from GD 6-9 and GD6-15 compared to controls. However, these effects subsided after cessation of treatment and body weight and food consumption for the overall gestational period (GD 6-21) were not significantly different between the high dose group and controls. There were no maternal findings at necropsy that were judged to be the result of treatment with Alcohols, C7-9 branched. For the most part, uterine implantation parameters were equivalent between the treated and control groups.

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Remarks, cont'd	<p>There were slight differences between the high dose group and the control group in the number of post-implantation losses and resorptions, however these differences were not statistically significant and were deemed to be due to the poor health of the dams.</p> <p>Mean fetal body weight was equivalent between treated and control fetuses of both sexes. Three low dose, two mid dose, and one high dose fetus were stunted. There were no statistically significant differences in mean skeletal ossification sites and in total or individual external, visceral, or skeletal malformations between control and treated groups. There were statistically significant increases in total fetuses with skeletal variations and in the incidence of hypoplastic skull bones in the high dose group when compared to controls. These findings were slightly higher than the historical control range of the lab and were not observed with litter-based analysis. Statistically significant increases in the number of lumbar ribs were observed in the middle and high dose groups. However, due to the lack of embryotoxicity observed in this study, these findings were attributed to maternal toxicity observed during treatment.</p>
Conclusions	Under the conditions of this study, Alcohols, C7-9 branched induces maternal toxicity at concentrations that are not embryotoxic.
Data Quality	1 - Reliable without restrictions
Reference	Exxon Biomedical Sciences, Inc. (1994). Developmental Toxicity Study in Rats, Unpublished report.
Date last changed	February, 2001

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Acute Toxicity

Test Substance CAS No.	Alkenes, C7-9, C8 rich 68526-54-5
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels:	NA Oral LD ₅₀ Pre-GLP 1975 Albino Rats Male 10 rats Oral gavage NA Single Treatment 5000 mg/kg
Control group and Treatment:	NA
Remarks on Test Conditions	A single dose of undiluted test material (5,000 mg/kg) was administered to male rats (not fasted). Individual body weights were recorded on Day 0 and Day 7. Gross necropsy examinations were performed on all animals that died or were killed.
Results (LD₅₀ or LC₅₀):	LD ₅₀ > 5000 mg/kg
Remarks	Hypoactivity and diarrhea were noted within 6-22 hours post-oral administration and subsided by the second post-oral exposure day. There were no significant findings observed during the gross necropsy examination.
Conclusions	Under the conditions of this study, Alkenes, C7-9, C8 rich have a low order of acute oral toxicity.
Data Quality	1 - Reliable without restrictions, comparable to a guideline study
Reference	Exxon Research and Engineering Company (1975). Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study. Unpublished Report.
Date last changed	October, 2000

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Acute Toxicity

Test Substance CAS No.	Alkenes, C7-9, C8 rich 68526-54-5
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:	NA Dermal LD ₅₀ Pre-GLP 1975 Albino rabbits Males and Females 2/sex/dose Dermal NA Single 24-hour exposure 200, 3160 mg/kg. NA
Remarks on Test Conditions	A single dermal application of the test material was made to four groups of four rabbits at doses of 200 and 3,160 mg/kg. The test material was applied to abraded skin. Individual body weights were recorded on Days 0, 7 and 14. Gross necropsies were performed at the end of the experiment.
Results (LD₅₀ or LC₅₀):	LD ₅₀ > 3,160 mg/kg
Remarks	There were no mortalities at any dosage level tested. Thus, the LD ₅₀ in albino rabbits is greater than the highest dose tested. Signs of erythema, mild to moderate edema and second degree burns were observed at 24 hours at both doses. At 7 and 14 days, focal escharosis was observed at the low dose. At the high dose, escharosis, fissuring, hemorrhaging, and wrinkling were observed at 7 days and escharosis was observed at 14 days. Necropsy examination revealed emaciation and depletion of fat stores in one male rabbit in the low dose group. No other gross pathologic alterations were observed.
Conclusions	Alkenes, C8-10, C9 rich have a low order of acute dermal toxicity.
Data Quality	1 - Reliable without restrictions
Reference	Exxon Research and Engineering Company (1975). Chemical Hazard Data Sheet on Octenes and Acute Oral Toxicity Study, Acute Dermal Toxicity Study, Eye Irritation Toxicity Test and Acute Vapor Inhalation Toxicity Study. Unpublished Report.
Date last changed	October, 2000

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:	Alkenes, C7-9, C8 rich 68526-54-5 NA Inhalation LC ₅₀ Pre-GLP 1977 Albino rats, mice, and guinea pigs Males 10/species Inhalation NA Single 6-hour Exposure 31.67 mg/L Control animals were exposed to clean air at the same flow rate as the treated group.
Remarks on Test Conditions	<p>Rats, mice, and guinea pigs received a single, 6-hour exposure to the test material. The exposure was conducted in a 1000-liter glass and stainless steel chamber. The compound was placed in a 2000 ml three-necked flask, pre-weighed and mounted outside the chamber. Air was bubbled through the test material at 5 L/min and was then combined with an additional airflow of 10 L/min to produce a total flow rate through the chamber of 15 L/min.</p> <p>All animals were observed for signs of toxicity, abnormal behavior, and mortality during the exposure period and for 14 days after the exposure. Necropsies were performed on all surviving animals and any animals that died during the exposure or post-exposure observation period.</p>
Results (LD₅₀ or LC₅₀):	LC₅₀ > 31.7 mg/L (rat) LC₅₀ > 31.7 mg/L (mouse) LC₅₀ < 31.7 mg/L (guinea pig)
Remarks	<p>There were no deaths in the air-exposed animals. In the treated animals, six guinea pigs and three rats died during the exposure period. No mice died during the study. One guinea pig died on Day 1 of the recovery period. All animals showed compound awareness 1 minute after exposure began and became increasingly agitated during the first 35 minutes of exposure. After 100 minutes, some animals were experiencing tremors and convulsions. Necropsy examination indicated dark red coloration of the lungs of 15 animals (3 rats, 4 mice, and 8 guinea pigs). Six guinea pigs had liver discolorations. Five guinea pigs showed pale kidney color also. One guinea pig that died showed a large amount of blood in the heart. Fifteen animals (7 rats, 6 mice, and 2 guinea pigs) showed no gross lesions.</p>
Conclusions	<p>Under conditions of this study, Alkenes, C7-9, C8 rich have a low order of acute inhalation toxicity in rats.</p>
Data Quality	<p>1 - Valid without restrictions; Comparable to a guideline study.</p>
Reference	<p>Exxon Corporation (1977). Acute Inhalation Toxicity- Rats, mice and guinea pigs. Unpublished Report.</p>
Date last changed	<p>October, 2000</p>

Acute Toxicity

Test Substance CAS No.	Alcohols, C8-10 iso, C9 rich 68526-84-1
Method/Guideline	NA
Type of Study	Acute oral toxicity
GLP	Pre-GLP
Year	1968
Species/strain	Rats/Sprague-Dawley
Sex	Males
No. of animals/sex/dose	5/dose
Route of administration	Gastric Intubation
Vehicle	None
Frequency of Treatment	Single Exposure
Dose/Concentration Levels	34.6, 120, 417, 1450, 5000 or 10,000 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	After a three to four hour fasting period, groups of 5 rats (approximately 252-295 grams) received the undiluted test material at doses of 34.6, 120, 417, 1450, 5000 or 10,000 mg/kg body weight. Observations were recorded immediately after dosing; at one, four and 24 hours; and once daily for a total of 14 days.
Results	LD ₅₀ = 2979 mg/kg
Remarks	No deaths occurred in the 34.6, 120, 417, and 1450 mg/kg groups throughout the study. Two of the five animals in the 5000 mg/kg group died within 24 hours and all of the animals in the 10,000 mg/kg group died within 24 hours. Depression, labored respiration and evidence of excessive urination and/or diarrhea were observed at the 5,000 and 10,000 mg/kg dose levels. These signs of toxicity were observed within one hour of administration. At necropsy, abscessed lungs, dark red lungs and a dark zone between the renal cortex and medulla were observed in animals from the 5,000 and 10,000 mg/kg dose levels.
Conclusions	Under conditions of this study, Alcohols, C8-10 iso, C9 rich have a low order of acute oral toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Esso Research and Engineering (1968). Unpublished report.
Date last changed	September, 2000

Acute Toxicity

Test Substance	Alcohols, C8-10 iso, C9 rich
CAS No.	68526-84-1
Method/Guideline	Other
Type of Study	Acute dermal toxicity
GLP	Pre-GLP
Year	1968
Species/strain	Rabbits/New Zealand White
Sex	Males and Females
No. of animals/sex/dose	2/sex/dose
Route of administration	Dermal
Frequency of Treatment	Single Exposure
Dose/Concentration Levels	50, 200, 794 and 3,160 mg/kg
Remarks on Test Conditions	A single application of the test material was made to four groups of four rabbits (2.0 to 2.8 kg) at doses of 50, 200, 794 and 3160 mg/kg. The material was applied to abraded abdominal skin under occlusive dressing. Observations were recorded immediately following application; at one, four and 24 hours; and once daily thereafter for a total of 14 days.
Results	LD ₅₀ > 3,160 mg/kg of body weight.
Remarks	No deaths were observed at any timepoint in this study. No evidence of systemic toxicity was observed. Dose-related moderate to severe skin irritation was produced. For all of the doses tested, no compound-related alterations were observed at necropsy.
Conclusions	Under the conditions of this study, Alcohols, C8-10 iso, C9 rich has a low order of acute dermal toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP)
Reference	Esso Research and Engineering (1968). Unpublished report.
Date last changed	September, 2000

Repeat Dose Toxicity

Test Substance CAS No.	Isononanol --
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of treatment Vehicle Statistical methods	Other 14-day repeated dose Not specified 1983 Rats /Wistar Male 5/treatment, 10/control; 1mmol/kg/day of isononanol (144 mg/kg/day) Oral gavage. Once daily for 14 days Polyethylene glycol 300 Mean values compared to controls by Student's t-test.
Remarks on Test Conditions	After acclimation for 1 week, five animals received 1mmol/kg/day (130 mg/kg/day) of the test substance by oral gavage and ten animals received only the vehicle, PEG 300, daily for 14 days. Animals were sacrificed after 14 days by halothane overdose and blood was withdrawn by cardiac puncture and analyzed for plasma cholesterol and triglycerides. The liver was removed for histopathological analysis, analysis of catalase, and CN-insensitive palmitoyl CoA oxidation. Testicular weight was also determined.
Results	NOAEL \geq 144 mg/kg/day
Remarks	Isononanol did not significantly change body weight gain, liver to body weight ratio, or testis to body weight ratio when compared to vehicle controls. Isononanol did not induce any changes in glycogen vacuolation or fat vacuolation. The levels of cholesterol and triglyceride were not significantly different between animals treated with isononanol and vehicle controls. There was a slight induction of palmitoyl CoA oxidase activity. However, the activity of other peroxisome-associated enzymes was not affected and overall peroxisome number was not effected. No hyperlipidemia was observed.
Conclusions	Under the conditions of this study, isononanol has a low order of sub-acute toxicity in male rats for the endpoints studied.
Data Quality	2 - Valid with restrictions. Not a guideline study.
Reference	C. Rhodes, T. Soames, M.D. Stonard, M.G. Simpson, A.J. Vernall, C.R. Elcombe, "The absence of testicular atrophy and in vivo and in vitro effects on hepatocyte morphology and peroxisomal enzyme activities in male rats following the administration of several alkanols," (1984). <u>Toxicology Letters</u> 21 : 103-109.
Date last changed	13-Sep-00

Developmental Toxicity

Test Substance CAS No.	Isononylalcohol 1 68515-81-1
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1989
Species/strain	Rats/Wistar
Sex	Females
No. of animals/ sex/dose	10/dose
Route of administration	Oral gavage
Vehicle	Aqueous emulsion in 0.005% Cremophor EL
Frequency of Treatment	Gestation days 6-15
Dose/Concentration Levels	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Control group and Treatment	Control Group 1: Doubly distilled water Control Group 2: Doubly distilled water with 0.005% Cremophor EL
Statistical Methods	Dunnett's test, Fisher's exact test
Remarks on Test Conditions	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononylalcohol 1 or Isononylalcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Results	NOAEL = 144 mg/kg/day (Maternal and Fetal)
Remarks	At the lowest dose level, no maternal toxicity was observed. There were an increased number of fetuses with hydronephrosis. However, the significance of this endpoint as an indicator of marginal developmental toxicity is questionable. At both the 144 and 720 mg/kg/day dose levels, there were no effects on the following parameters: uterine weight, conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, and viable fetuses. At the 720 mg/kg/day level, the following signs of maternal toxicity were observed - reduced food consumption, reduced body weight, unsteady gait, and reddish nasal discharge. Fetal effects included a slightly reduced mean fetal body weight and an increased number of fetuses with hydronephrosis. Signs of maternal toxicity at the 1440 mg/kg/day level included reduced food consumption and mean body weight, severe clinical symptoms like abdominal or lateral position, and unsteady gait. In addition, 7 of the animals found dead by gestation day 11 and the remaining 3 were sacrificed in moribund condition by gestation day 10. At necropsy, all animals had light brown-gray discoloration of the liver and some had evidence of lung edema and petechiae in the lungs. Because of the death of all dams within the high dose group, no data were available to assess uterus weight, reproduction parameters, or fetal effects.

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Conclusions	When administered by oral gavage under the conditions of this study, Isononylalcohol 1 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononylalcohol 1 does not alter reproductive parameters at doses that are not maternally toxic.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247.
Date last changed	February, 2001

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Developmental Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals Route of administration Frequency of Treatment Dose/Concentration Levels Control Group and Treatment</p> <p>Statistical methods</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p>	<p>Isononyl alcohol 2 68515-81-1</p> <p>OECD 414 Developmental Toxicity Yes 1989 Rats/Wistar Females 10/group Oral gavage Gestation days 6-15 144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day) Control Group 1: Doubly distilled water Control Group 2: Doubly distilled water with 0.005% Cremophor EL Dunnett's test, Fisher's exact test</p> <p>The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isononyl alcohol 1 or Isononyl alcohol 2 were administered to rats (10/dose) on days 6 through 15 of gestation at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.</p> <p>NOAEL = 144 mg/kg/day</p> <p>At the lowest dose level, no maternal or fetal toxicity was observed. In addition, there were no changes in reproductive parameters. At the 720 mg/kg/day level, signs of maternal toxicity included unsteady gait, piloerection, salivation, and reduced body weight gain and food consumption. There was also an increased frequency of fetuses with hydronephrosis at this level. At this level, there were no significant changes in reproductive parameters. Although there was an increased number of late resorptions, this number was within the range of biologic variation, was not dose-dependent, and was therefore considered incidental.</p> <p>At the highest dose level, dams exhibited marked decreases in weight gain and food consumption, and displayed severe clinical symptoms, including unsteady gait, apathy, and abdominal or lateral position. One animal was found dead on gestation day 9 and two other dams were sacrificed in moribund condition on gestation days 8 and 109. At necropsy, light brown-gray discoloration of the liver, lung edema, and petechiae in the lungs, heart, or bladder were observed. Fetuses from the high dose group had markedly reduced mean fetal body weight, increased frequency of hydronephrosis, and a higher frequency of fetuses with skeletal variations and retardations. At the highest dose, there were no changes in fertility parameters.</p>
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Conclusions	When administered by oral gavage under the conditions of this study, Isononylalcohol 2 causes embryo/fetal toxicity at doses that induce overt maternal toxicity. In addition, Isononyl alcohol 2 does not alter fertility parameters at doses that are not maternally toxic.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isononylalcohol 1 and Isononylalcohol 2 in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000247.
Date last changed	February, 2001

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Developmental Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of treatment Dose/Concentration Levels Control group and treatment Statistical methods</p> <p>Remarks on Test Conditions</p>	<p>1-Nonanol --</p> <p>Other Developmental Toxicity Not specified 1989 Rats/Sprague-Dawley Pregnant females 15 dams/dose Inhalation 7 hrs/day; Gestation days 1-19 150 mg/m³ (Saturated vapors) 15 sham-exposed rats MANOVA, ANOVA, Kruskal-Wallis test</p> <p>Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Exposures were conducted in Hinners-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance, which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 3500 mg/m³. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO₂ asphyxiation, and the uterus and ovaries were removed and examined for corpora lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.</p>
<p>Results</p>	<p>NOAEL = 150 mg/m³</p>
<p>Remarks</p>	<p>No treatment-related effects were observed in dams. There were no statistically significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. There were no statistically significant differences between the mean number of corpora lutea and resorptions, the sex ratio, and the mean fetal weights between the control and treated groups.</p>

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Conclusions	Under the conditions of this study, exposure of pregnant rats to saturated vapors of 1-Nonanol does not induce maternal or fetal toxicity.
Data Quality	2 - Reliable with restrictions - Similar to guideline study; only one exposure level.
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) <u>Journal of the American College of Toxicology</u> 9(1) : 93-97. NIOSH, Division of biomedical and behavioral sciences
Date last changed	February, 2001

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Dose/Concentration Levels	C ₉ HOF Other Acute Oral Yes 1985 Rats M/F 5/sex/dose Oral NA 5000 mg/kg
Remarks on Test Conditions	<p>Animals were fasted approximately 18 hours prior to administration of the test material. Undiluted test material was administered by oral intubation. The dose administered was calculated by dividing the dose level by the density to arrive at the dose volume. The animal's body weight was then multiplied by the dose volume to arrive at the animal's actual dose. Animals were examined for viability as well as the nature, onset, severity, and duration of toxicological signs at 1,2,4, and 6 hours after dosing, and once per day thereafter for a total of 14 days. Body weights were recorded the day prior to dosing, on Day 0 and Days 7 and 14. On day 14, animals were weighed and sacrificed. Gross necropsies were performed on all animals by qualified personnel.</p>
Results	LD ₅₀ > 5000 mg/kg
Remarks	<p>All animals survived to study termination. The animals displayed an increase in body weight over the study period. In-life observations were minimal and included staining of the anogenital area in some animals. Nine of the ten animals exhibited no observable abnormalities through the second week of the study. Upon postmortem examination, slightly discolored lungs, maloccluded incisors, slight alopecia, and red staining around the eye were observed in two of the animals. Eight of the ten test animals exhibited no observable abnormalities at necropsy.</p>
Conclusions	Under the conditions of this study, C ₉ HOF has a low order of acute oral toxicity.
Data Quality	1 - Reliable without restrictions
Reference	"Acute oral toxicity study in the rat," (1985) performed by Bio/dynamics Inc. for Exxon Biomedical Sciences Inc.
Date last changed	October, 2001

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Dose/Concentration Levels	C ₉ HOF Other Acute Dermal Yes 1985 Rabbit M/F 3/sex/dose Dermal NA 3160 mg/kg
Remarks on Test Conditions	<p>Test material was applied as a single dose to the clipped backs of rabbits. The test material remained in contact with the intact skin of all animals for a period of 24 hours. The test material was covered with a gauze patch and secured with tape. To prevent evaporation or ingestion of the test material, the gauze patch was secured to the trunk of the animal with tape and a plastic sleeve. The amount of material remaining on the skin of each animal after the 24 hour exposure was estimated. Animals were observed for clinical signs 2 and 4 hours after dosing and once per day thereafter for a total of 14 days. Dermal responses were evaluated 24 hours after topical application and on 3, 7, 10, and 14 days according to the Draize method of scoring. Body weights were recorded on the day of dosing, and Days 7 and 14. After the two weeks, all animals were sacrificed and gross necropsies were performed.</p>
Results	LD ₅₀ > 3160 mg/kg
Remarks	<p>There were no deaths prior to study termination. At study termination, all animals displayed an increase in body weight over their initial body weights. Clinical in-life observations were minimal and included nasal discharge, abdominal staining, staining in the anogenital area, thin hair coat, soft stool, and alopecia. Gross necropsy revealed single incidences of anogenital staining, thin hair coat, and alopecia. Three of the six test animals exhibited no observable abnormalities. Dermal observations included well-defined to moderate-to-severe erythema and slight edema at 72 hours. However, irritation decreased by Day 14 and only slight erythema and edema were observed in one animal by Day 14. The remaining animals showed no signs of irritation by Day 14.</p>
Conclusions	<p>Under the conditions of this study, C₉HOF has a low order of acute toxicity by the dermal route of exposure.</p>
Data Quality	1 - Reliable without restrictions.
Reference	"Acute dermal toxicity study in the rabbit," (1985) Bio/dynamics, Inc. for Exxon Biomedical Sciences Inc.
Date last changed	October, 2001

Acute Toxicity

Test Substance CAS No.	Alkenes, C8-10, C9 rich 68526-55-6
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels:	NA Oral LD ₅₀ Pre-GLP 1957 Rats/Holtzman Male 5/dose Oral gavage 0.5% aqueous methyl cellulose solution Single Treatment 0.1, 1.0, and 10.0% volume/volume in a 0.5% aqueous methyl cellulose solution. (Equivalent to 7.4, 23.3, 73.8, 233, 738, 2332 mg/kg)
Control group and Treatment:	For comparison, untreated animals were necropsied at the end of the study.
Remarks on Test Conditions	Prior to dosage, food was withheld from the animals for three hours. Following exposure, food and water were available at all times. The animals were observed for gross effects and mortality several times on the day of exposure and once daily thereafter for 7 days. Gross necropsies were performed at the end of the observation period.
Results (LD₅₀ or LC₅₀):	LD ₅₀ > 2332 mg/kg
Remarks	No mortalities were observed at any of the doses tested. Animals in the high dose group appeared slightly depressed the day after administration of the test material. For several hours following exposure, the animals in the high dose group also showed slight nasal discharge. Otherwise, all animals appeared normal throughout the study. Animals in all groups exhibited normal weight gain. Gross necropsy did not reveal any abnormalities other than slightly congested adrenal glands in animals from the three higher dose levels (233, 738, and 2332 mg/kg).
Conclusions	Under the conditions of this study, Alkenes, C8-10, C9 rich have a low order of toxicity.
Data Quality	2 - Reliable with restrictions, comparable to a guideline study (pre-GLP).
Reference	Hazleton Laboratories for Esso Research and Engineering Co., Acute Oral Administration, 1957.
Date last changed	October, 2000

Acute Toxicity

Test Substance CAS No.	Alkenes, C8-10, C9 rich 68526-55-6
Method/Guideline	NA
Type of Study	Dermal LD ₅₀
GLP	Pre-GLP
Year	1957
Species/strain	Albino rabbits
Sex	Males
No. of animals/sex/dose	4/dose
Route of administration	Dermal
Vehicle	NA
Frequency of Treatment:	Single 24-hour exposure
Dose/Concentration Levels:	73.8, 233, 738, 2332 mg/kg.
Control group and Treatment:	NA
Remarks on Test Conditions	Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually.
Results (LD₅₀ or LC₅₀):	LD₅₀ > 2332 mg/kg
Remarks	No mortalities were observed at any dose tested. The abdomens and binders were dry at the end of the exposure period, indicating a good rate of dermal absorption of the applied material. The test material produced mild dermal irritation characterized by mild erythema. Most of the animals showed slight atonia for several days of the observation period and desquamation during the final two days of the observation period. Throughout the study, all animals exhibited normal appearance and behavior. Body weight gain was normal throughout the study. There were no significant findings at necropsy.
Conclusions	Alkenes, C8-10, C9 rich have a low order of acute dermal toxicity.
Data Quality	2 - Reliable with restrictions. Pre-GLP.
Reference	Hazleton Laboratories for Esso Research and Engineering Co., Acute Dermal Application, 1957.
Date last changed	October, 2000

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Acute Toxicity

<p> Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment: </p>	<p> Alkenes, C8-10, C9 rich 68526-55-6 Other Inhalation LC₅₀ Not specified 1977 CD-1 Mice, Sprague-Dawley Rats, Hartley Guinea Pigs Males and Females 5/sex/species Inhalation NA Single Dose 11.1 mg/L for 6 hours Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group. </p>
<p>Remarks on Test Conditions</p>	<p>An airstream was bubbled through the test material at a rate of 33.1 L/min and passed through a 760 L test chamber containing the test animals for a total of 6 hours. Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Body weights were recorded on Days 0, 1, 2, 4, 7, and 14. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study.</p>
<p>Results (LD₅₀ or LC₅₀):</p>	<p>LC₅₀ > 11.1 mg/L for 6 hours</p>
<p>Remarks</p>	<p>None of the animals died during the exposure period or during the 14-day post-exposure observation period. A total of 132.1 g of test material was delivered to the chamber during the course of the exposure. The overall nominal concentration of the test substance was 11.1 mg/L. During the last 4 hours of exposure, mice exhibited labored breathing patterns, rats exhibited limb ataxia and generally lethargic behavior, and the guinea pigs showed slight tremors. No similar signs were noted in the control animals, indicating that these effects were due to exposure to the test substance. However, all of the symptoms subsided as the test chamber was cleared with clean air. On day 4 of the post-exposure observation period, one of the exposed mice had tremors, but the symptoms only occurred on that day and were not believed to be due to exposure to the test substance. Signs of toxicity observed during the 14-day post-exposure period included dry rales, soft stool, and nasal discharge in rats, however, these signs were observed in both the exposed and control animals and are not believed to be due to the test substance. In both exposed animals and controls, there was a slight decrease in body weight during the first few days following exposure, after which the animals recovered their normal body weight. There were no significant differences observed between the exposed animals and the test animals at necropsy. Although there was a high incidence of kidney lesions in both groups of guinea pigs, the rate was slightly higher in the exposed animals than in the controls. However, the difference was not statistically significant.</p>
<p>Conclusions</p>	<p>Under conditions of this study, Alkenes, C8-10, C9 rich have a low order of acute inhalation toxicity in rats.</p>
<p>Data Quality</p>	<p>2 - Valid with restrictions. No analysis of exposure atmosphere.</p>
<p>Reference</p>	<p>"An Acute Inhalation Toxicity Study of MRD-76-57 in the Mouse, Rat, and Guinea Pig," Bio/dynamics, Inc. for Exxon Research and Engineering Company, April 11, 1977.</p>
<p>Date last changed</p>	<p>October, 2000</p>

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Genetic Toxicity

Test Substance CAS No.	Alkenes, C8-10, C9 rich 68526-55-6
Method Type of Study GLP Year Species/Strain	EPA OTS 798.5395 Mouse Micronucleus Yes 1991 Mouse/ B6C3F1
Sex Number/sex/dose Route of administration Vehicle Exposure Period Concentrations	Male and Female 15/sex Oral gavage NA Single dose 1.25, 2.5, and 5 g/kg. Concentrations were based on the results of a range-finding study.
Controls	Positive: Cyclophosphamide (40 mg/kg) Negative: Corn oil
Statistical Methods	Analysis of variance (ANOVA), Duncan's Multiple Range Test
Remarks on Test Conditions	The test material and the carrier were administered by oral gavage as a single dose to mice (not fasted). The positive control, cyclophosphamide, was administered by intraperitoneal injection as a single dose. Animals from the appropriate groups were sacrificed by carbon dioxide asphyxiation at appropriately 24, 48 and 72 hours after dose administration. Animals dosed with cyclophosphamide were sacrificed at 24 hours only. Immediately upon sacrifice, the bone marrow was removed from both femurs of each animal, resuspended, and prepared for microscopy. Samples were blindly coded and stained with acridine orange.
<u>Results</u>	Negative
Remarks for Results	There was no statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. Thus, the test material was not clastogenic. The positive control induced a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes, which indicates that the positive control is clastogenic. The test material did not induce a statistically significant increase in the mean number of micronucleated polychromatic erythrocytes. However, the test material did induce a significant decrease in polychromatic erythrocytes in both males and females at 48 and 72 hours when treated with the high dose. In addition, there was a statistically significant difference in the mean percent of polychromatic erythrocytes in the high dose group at 48 and 72 hours and in the mid dose group at 48 hours. These observations indicate that the test material was toxic to mouse bone marrow at higher concentrations, but did not induce micronuclei formation.
Conclusions	Under conditions of this assay, the test material is not considered clastogenic in mice up to and including 5.0 g/kg when evaluated up to 72 hours after dose administration.
Data Quality	1 - Reliable without restrictions
Reference	"In vivo mammalian bone marrow micronucleus assay: oral gavage method," Exxon Biomedical Sciences, Inc. 1991.
Date last changed	October, 2000

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Genetic Toxicity

Test Substance CAS No.	Alkenes, C8-10, C9 rich 68526-55-6
Method/Guideline Test Type GLP Year	EPA OTS 798.5265 Ames Assay Yes 1991
Species/strain	Salmonella typhimurium; TA98; TA100; TA1535; TA1537; TA1538
Metabolic Activation	With and without S9 fraction of livers from rats pretreated with Aroclor 1254.
Dose/Conc. Levels	10, 32, 100, 320, and 1000 µg/plate
Statistical methods	The mean plate count and standard deviation for each dose point were determined. Any test value that was equal to or greater than three times the mean value of the concurrent vehicle control was considered to be a positive dose.
Remarks on Test Conditions	
Solvent:	DMSO was used for controls; Ethanol was used for the test material
Positive Controls:	2-Aminoanthracene, 9-Aminoacridine, 2-Nitrofluorene, N-methyl-N-nitro-N-nitrosoguanidine
Negative Controls:	Vehicle controls were dosed at 0.1 ml/plate ethanol and 0.1 ml/plate DMSO
	To determine the highest dose of compound to be used in the assay, a dose range from 1 to 10,000 µg/plate was tested. Only strain TA98 was used. The toxicity pretest was repeated and toxicity was observed as a reduction in both background and revertant colony counts. 1000 µg/plate was selected as the high dose to be used on the mutagenesis assay for both the saline (-S9) and the +S9 treated plates.
	A repeat assay was performed in order to verify the data produced in the initial assay.
<u>Results</u>	Negative
Remarks	The test material did not produce any evidence of mutagenicity. Doses were considered positive if test values were equal to or greater than 3X the mean value of the vehicle control. In the initial and repeat assays, neither a positive response nor a dose related increase in revertants was observed for any of the tester strains either in the presence or absence of metabolic activation. All other positive and negative controls responded in a manner consistent with data from previous assays.
Conclusions	Under conditions of this assay, the test material was not mutagenic for the <i>Salmonella</i> tester strains at doses up to and including 1000 µg/plate.
Data Quality	1 - Valid without restrictions
Reference:	Microbial Mutagenesis in <i>Salmonella</i> : Mammalian Microsome Plate Incorporation Assay; Exxon Biomedical Sciences Inc., 1991.
Date last changed	November, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Dose/Concentration Levels:	C ₁₀ V-HOF -- Other Acute Oral Yes 1985 Rats M/F 5/sex/dose Oral NA 5000 mg/kg
Remarks on Test Conditions	<p>Animals were fasted approximately 18 hours prior to administration of the test material. Undiluted test material was administered by oral intubation. The dose administered was calculated by dividing the dose level by the density to arrive at the dose volume. The animal's body weight was then multiplied by the dose volume to arrive at the animal's actual dose.</p> <p>Animals were examined for viability as well as the nature, onset, severity, and duration of toxicological signs at 1,2,4, and 6 hours after dosing, and once per day thereafter for a total of 14 days. Body weights were recorded the day prior to dosing, on Day 0 and Days 7 and 14. On day 14, animals were weighed and sacrificed. Gross necropsies were performed on all animals by qualified personnel.</p>
Results	LD ₅₀ > 5000 mg/kg
Remarks	<p>All animals survived to study termination. The animals displayed an increase in body weight over the study period. In-life observations were minimal and included staining of the anogenital area and soft stool in some animals. By Day 12, all animals exhibited no observable abnormalities. Gross postmortem examination revealed no observable abnormalities in any animals.</p>
Conclusions	<p>Under the conditions of this study, C₁₀V-HOF has a low order of acute oral toxicity.</p>
Data Quality	1 - Reliable without restrictions.
Reference	<p>"Acute oral toxicity study in the rat," (1985) performed by Bio/dynamics Inc. for Exxon Biomedical Sciences Inc.</p>
Date last changed	October, 2001

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Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Dose/Concentration Levels:	C ₁₀ U-HOF -- Other Acute Oral Yes 1985 Rats M/F 5/sex/dose Oral NA 5000 mg/kg
Remarks on Test Conditions	<p>Animals were fasted approximately 18 hours prior to administration of the test material. Undiluted test material was administered by oral intubation. The dose administered was calculated by dividing the dose level by the density to arrive at the dose volume. The animal's body weight was then multiplied by the dose volume to arrive at the animal's actual dose. Animals were examined for viability as well as the nature, onset, severity, and duration of toxicological signs at 1,2,4, and 6 hours after dosing, and once per day thereafter for a total of 14 days. Body weights were recorded the day prior to dosing, on Day 0 and Days 7 and 14. On day 14, animals were weighed and sacrificed. Gross necropsies were performed on all animals by qualified personnel.</p>
Results	LD ₅₀ > 5000 mg/kg
Remarks	<p>All animals survived to study termination. The animals displayed an increase in body weight over the study period. In-life observations were minimal and included staining of the anogenital area in some animals. By Day 6, all animals exhibited no observable abnormalities. Gross postmortem examination revealed slight lung discoloration in three animals and no observable abnormalities in the other seven animals.</p>
Conclusions	<p>Under the conditions of this study, C₁₀U-HOF has a low order of acute oral toxicity.</p>
Data Quality	1 - Reliable without restrictions.
Reference	<p>"Acute oral toxicity study in the rat," (1985) performed by Bio/dynamics Inc. for Exxon Biomedical Sciences Inc.</p>
Date last changed	October, 2001

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Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Dose/Concentration Levels	C ₁₀ V-HOF -- Other Acute Dermal Yes 1985 Rabbit M/F 3/sex/dose Dermal NA 3160 mg/kg
Remarks on Test Conditions	<p>Test material was applied as a single dose to the clipped backs of rabbits. The test material remained in contact with the intact skin of all animals for a period of 24 hours. The test material was covered with a gauze patch and secured with tape. To prevent evaporation or ingestion of the test material, the gauze patch was secured to the trunk of the animal with tape and a plastic sleeve. The amount of material remaining on the skin of each animal after the 24 hour exposure was estimated. Animals were observed for clinical signs 2 and 4 hours after dosing and once per day thereafter for a total of 14 days. Dermal responses were evaluated 24 hours after topical application and on 3, 7, 10, and 14 days according to the Draize method of scoring. Body weights were recorded on the day of dosing, and Days 7 and 14. After the two weeks, all animals were sacrificed and gross necropsies were performed.</p>
Results	LD ₅₀ > 3160 mg/kg
Remarks	<p>There were no deaths prior to study termination. Five of six animals displayed an increase in body weight over their initial values, while the remaining animal displayed a slight loss in body weight. Clinical in-life observations were minimal during the study and included soft stool, nasal discharge, anogenital staining, ocular discharge, and alopecia. Gross necropsy revealed discoloration of the kidneys in one animal, salivary glands abnormalities in one animal, and desquamation in two animals. Three of the six test animals exhibited no observable abnormalities at necropsy. The test material produced some dermal irritation, including desquamation. However, by Day 14, only one animal displayed very slight erythema and edema.</p>
Conclusions	<p>Under the conditions of this study, C₁₀V-HOF has a low order acute toxicity by the dermal route of exposure.</p>
Data Quality	1 - Reliable without restrictions.
Reference	"Acute dermal toxicity study in the rabbit," (1985) Bio/dynamics, Inc. for Exxon Biomedical Sciences Inc.
Date last changed	October, 01

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Dose/Concentration Levels	C ₁₀ U-HOF Other Acute Dermal Yes 1985 Rabbit M/F 3/sex/dose Dermal NA 3160 mg/kg
Remarks on Test Conditions	<p>Test material was applied as a single dose to the clipped backs of rabbits. The test material remained in contact with the intact skin of all animals for a period of 24 hours. The amount of material remaining on the skin of each animal after the 24 hour exposure was estimated. Animals were observed for clinical signs 2 and 4 hours after dosing and once per day thereafter for a total of 14 days. Dermal responses were evaluated 24 hours after topical application and on 3, 7, 10, and 14 days according to the Draize method of scoring. Body weights were recorded on the day of dosing, and Days 7 and 14. After the two weeks, all animals were sacrificed and gross necropsies were performed.</p>
Results	LD ₅₀ > 3160 mg/kg
Remarks	<p>There were no deaths prior to study termination. All animals displayed an increase in body weight over the course of the study. Clinical in-life observations during the study were minimal. One animal that was observed with its collar in its mouth at three consecutive observations intervals exhibited ataxia, nasal discharge, decreased food consumption, emaciation, staining in the anogenital area, a small amount of stool, alopecia, scabs, and maloccluded incisors. This animal had its collar removed for the remainder of the study. Necropsy revealed maloccluded incisors in 1 animal and 3 animals with alopecia. Three of the 6 test animals exhibited no observable abnormalities. Dermal observations included initial moderate-to-severe erythema that diminished in severity by the end of the observation period. Two animals displayed fissuring and all animals displayed atonia and desquamation.</p>
Conclusions	Under the conditions of this study, C ₁₀ U-HOF has a low order acute toxicity by the dermal route of exposure.
Data Quality	1 - Reliable without restrictions
Reference	"Acute dermal toxicity study in the rabbit," (1985) Bio/dynamics, Inc. for Exxon Biomedical Sciences Inc.
Date last changed	October, 2001

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Alcohols, C9-C11 iso, C10 rich 68526-85-2
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment Dose/Concentration Levels	Other Acute oral toxicity Pre-GLP 1960 Rats/Sprague-Dawley Male 5/dose Oral gavage Corn oil Single Treatment 0.1, 1.0, 10.0, 30.0% volume/volume emulsion in corn oil (Equivalent to 26, 82, 260, 820, 2600, 8200 mg/kg)
Control group and Treatment	For comparison, untreated animals were necropsied at the end of the study.
Remarks on Test Conditions	Prior to dosage, food was withheld from the animals for three to four hours. The animals were observed for gross effects and mortality at one, four, and twenty-four hours, and once daily thereafter up until seven days. Gross necropsies were performed at the end of the observation period and samples of liver, kidney, brain, and blood were taken from untreated control animals and from all surviving animals at the 820 and 2600 mg/kg dose levels.
Results	LD ₅₀ = 4626 mg/kg
Remarks	<p>5/5 animals died within the first four hours following exposure to 8200 mg/kg. Animals in all other dose groups survived until the end of the study. At the one and four-hour intervals, animals in the 260 and 820 mg/kg dose groups were inactive and displayed labored respiration, ataxia, and sprawling of the limbs. At the 24-hour interval, animals had oily fur. After approximately 48-hours after dosing, most animals in these groups returned to normal appearance and behavior. At the 2600 mg/kg dose level, animals exhibited similar symptoms as above but also showed lacrimation and depressed righting and placement reflexes. Animals in this dose group also returned to normal appearance and behavior after 24 hours. At the highest dose, animals initially exhibited labored respiration, ataxia, and sprawling of the limbs, which was followed by a comatose state and death within 4 hours of exposure.</p> <p>The surviving animals at the five lower dose levels (26, 82, 260, 820, 2600 mg/kg) had weight gain that was within the normal range. Gross autopsies performed on animals that died (5/5 in 8200 mg/kg group) revealed congested lungs, kidneys, and adrenals, and dark-appearing spleens. No abnormalities were observed in the surviving animals at necropsy. Therefore, a histopathologic analysis was not performed.</p>
Conclusions	Under the conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of toxicity.
Data Quality	2 - Valid with restrictions (Pre-GLP).
Reference	Esso Research and Engineering (1960). Unpublished report.
Date last changed	October, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Alcohols, C9-C11 iso, C10 rich 68526-85-2
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals Route of administration Frequency of Treatment Dose/Concentration Levels	Other Acute dermal toxicity Pre-GLP 1960 Rabbits/Albino Males and Females 2/sex/dose Dermal Single Dose 80, 260, 820, and 2600 mg/kg
Remarks on Test Conditions	A single application of the test material was given to four groups (2/sex/dose) of four rabbits at doses of 80, 260, 820, and 2600 mg/kg. The material was applied under occlusive dressing to intact abdominal skin. Observations were recorded at one, four and 24 hours; and once daily thereafter for a total of 7 days. Samples of liver, kidney, brain and blood were taken from four untreated control albino rabbits and from each surviving animal at the 820 and 2600 mg/kg dose level.
Results	The acute dermal LD50 is > 2600 mg/kg
Remarks	No deaths were observed during this study. Mild to moderate erythema and edema were observed in animals at the three lower dose levels. Marked erythema and edema were observed at the highest dose level. Edema in each animal subsided within 3 days. Erythema in animals at the high dose group diminished in intensity but did not subside completely during the observation period. Autopsies performed following sacrifice revealed no gross pathological findings in any animal. Therefore, a histopathologic analysis was not performed.
Conclusions	Under conditions of this study, Alcohols, C9-C11 iso, C10 rich has a low order of acute dermal toxicity in rats.
Data Quality	2 - Valid with restrictions (Pre-GLP).
Reference	Esso Research and Engineering (1960). Unpublished report.
Date last changed	September, 2000

Robust Summaries - Olefin Hydroformylation Products

Developmental Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of treatment Dose/Concentration Levels Statistical methods</p> <p>Remarks on Test Conditions</p>	<p>Isodecanol 25339-17-7</p> <p>OECD 414 Developmental Toxicity Yes 1989 Wistar rats Females 10/dose Oral gavage Gestation day 6-15 158, 790, 1580 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day) Dunnett's test, Fisher's exact test</p> <p>The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isodecanol was administered at doses of 158, 790, or 1580 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.</p>
<p>Results</p>	<p>Maternal NOAEL = 158 mg/kg, Fetal NOAEL = 790 mg/kg</p>
<p>Remarks</p>	<p>At the lowest dose level, no adverse effects were observed in the dams or the fetuses as a result of exposure to the test compound. There were also no differences from controls with respect to the following reproductive parameters: conception rate, mean number of corpora lutea and implantation sites, pre- and post-implantation loss, number of resorptions, number of viable fetuses, placental weight, and sex distribution of the fetuses.</p> <p>Dams of the middle dose group exhibited reduced body weight gain and did not consume as much food as the control animals. Animals in the middle dose group also had an unsteady gait and reddish nasal discharge. No embryo or fetotoxic effects were observed at this dose. In addition, there were no changes in fertility parameters at the middle dose.</p> <p>Treatment with the highest dose of isodecanol resulted in statistically significant decreases in food consumption, body weight, and body weight gain in the dams. Three animals in the high dose group were found dead on gestation days 9 and 10. A fourth dam was sacrificed in moribund condition on gestation day 10. All of the dams in the high dose group had clinical symptoms that included nasal discharge, salivation, and signs of CNS depression.</p>

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Results, continued	At necropsy, the liver was light brown-gray and the mean gravid uterus weight was reduced. The lungs displayed signs of edema and emphysema. There were statistically significant increases in the number of resorptions in the high dose group as well as significantly reduced mean fetal body weight. However, there were no other statistically significant changes in reproductive parameters. Two litters had 2 anedeous fetuses. In addition, there were an increased number of fetuses with skeletal retardations.
Conclusions	Isodecanol is embryo and fetotoxic at doses that produce overt toxicity in the dam. In the absence of maternal toxicity, isodecanol is not embryo or fetotoxic under the conditions of this study. Furthermore, isodecanol does not alter fertility parameters at doses that are not maternally toxic.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-91000245.
Date last changed	October, 2000

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Developmental Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Frequency of treatment Dose/Concentration Levels Control group and treatment Statistical methods</p> <p>Remarks on Test Conditions</p>	<p>1-Decanol --</p> <p>Other Developmental Toxicity Not specified 1989 Sprague-Dawley Rats Pregnant females 15 dams/treatment Inhalation 7 hrs/day; Gestation days 1-19 100 mg/m³ (Saturated vapors) 15 sham-exposed rats MANOVA, ANOVA, Kruskal-Wallis test</p> <p>Throughout the study, all animals were housed under standard environmental conditions and allowed free access to food and water except when the pregnant females were in the exposure chamber. Following mating, sperm-positive females were placed in cages and weighed. Dams were weighed daily for the first week of exposure and weekly thereafter. Animals had free access to food and water. Exposures were conducted in Hinnert-type chambers. The purity of the test substance was ≥ 99% as measured by gas chromatography. A constant flow of the test substance was mixed with a known volume of heated compressed air, resulting in instantaneous vaporization of the test substance which then flowed into the chamber. The concentration of the test substance was monitored continuously and recorded every hour. Calibration checks were completed daily. Exposure concentrations were verified on a weekly basis using a secondary method of analysis. The highest concentration of vapor that could be generated was 100 mg/m³. Dams were exposed from days 1-19 of gestation. On day 20, dams were sacrificed by CO₂ asphyxiation, and the uterus and ovaries were removed and examined for corpora lutea, implantations, resorption sites, and live fetuses. Fetuses were removed and examined for external malformations, sexed, weighed, and examined for visceral or skeletal defects.</p>
<p>Results</p>	<p>NOAEL = 100 mg/m³</p>
<p>Remarks</p>	<p>No treatment-related effects were observed in dams. There were no significant differences in maternal weight gain, feed consumption, and water intake between the control and treated groups. In addition, no signs of fetal toxicity were observed. The number of corpora lutea and resorptions, the sex ratio, and fetal weights were not significantly different between the control and treated groups.</p>

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Conclusions	Under the conditions of this study, exposure of pregnant rats to vapors of 1-Decanol does not induce maternal or fetal toxicity.
Data Quality	2 - Reliable with restrictions - Similar to guideline study; only one exposure level.
Reference	B.K. Nelson, W.W. Brightwell, A. Khan, E.F. Krieg, Jr., A.M. Hoberman, "Developmental toxicology assessment of 1-Octanol, 1-Nonanol, and 1-Decanol administered by inhalation to rats." (1990) <u>Journal of the American College of Toxicology</u> 9(1) : 93-97. NIOSH, Division of Biomedical and Behavioral Sciences
Date last changed	February, 2001

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Developmental Toxicity

Test Substance	C7-9-11 Alcohol The test material consists mainly of linear alcohols and also contains significant amounts of alpha-methyl branched alcohols ranging in carbon chain length from C7 to C11.
CAS No.	85566-14-9
Method/Guideline	OECD 414
Type of Study	Developmental Toxicity
GLP	Yes
Year	1989
Species/strain	Rats/Wistar
Sex	Females
No. of animals/sex/dose	10/dose
Route of administration	Oral gavage
Frequency of treatment	Gestation day 6-15
Dose/Concentration Levels	144, 720, 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day)
Statistical methods	Dunnett's test, Fisher's exact test
Remarks on Test Conditions	The study was conducted according to OECD 414 guidelines except that 10 animals instead of the recommended 20 per group were employed. Isodecanol was administered at doses of 144, 720, or 1440 mg/kg/day (equivalent to 1, 5, and 10 mmol/kg/day). A standard dose volume of 5 ml/kg was used. Control group 1 was dosed with doubly distilled water. Control group 2 was dosed with emulsifier (doubly distilled water with 0.005% Cremophor EL). The state of health of the animals was monitored daily and food consumption and body weights of the animals were recorded regularly. Females were sacrificed on gestation day 20. Fetuses were removed and evaluated for sex, weight, and any external, soft tissue, or skeletal findings.
Results	Maternal NOAEL \geq 1,440 mg/kg/day Fetal NOAEL \geq 1,440 mg/kg/day
Remarks	No adverse effects were observed at any dose of C7-9-11 Alcohol. This included changes in body weight and food consumption by the dams, reproductive parameters, and signs of fetal toxicity.
Conclusions	C7-9-11 Alcohol does not produce signs of toxicity in the dam or the fetus. C7-9-11 Alcohol is not embryo or fetotoxic under the conditions of this study.
Data Quality	2 - Reliable with restrictions - Only 10 animals instead of the recommended 20 per group (OECD 414) were employed.
Reference	Report: Study of the Prenatal Toxicity of Isodecanol, 2-Ethylhexanol, and 711 Alcohol (T.C.) in Rats After Oral Administration (Gavage); EPA OTS Doc #: 89-910000245.
Date last changed	June, 2001

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Acute Toxicity

Test Substance CAS No.	Alcohols, C11-14 iso, C13 rich 68526-86-3
Method/Guideline	OECD 401
Type of Study	Acute oral toxicity
GLP	Yes
Year	1988
Species/strain	Rats/Wistar
Sex	Males and Females
No. of animals/sex/dose	5/sex/dose
Route of administration	Oral Gavage
Vehicle	None
Frequency of Treatment	Single Dose
Dose/Concentration Levels	2000 mg/kg
Control group and Treatment	None
Remarks on Test Conditions	The testing procedure used in this study is in accordance with OECD Guidelines 401. After being fasted for 12 to 18 hours, male and female rats were administered a single oral gavage dose of 2,000 mg/kg of the test article. Observations were made four times on day 1; and daily for 14 days. Animals were necropsied at the termination of the study.
Results	LD ₅₀ > 2,000 mg/kg.
Remarks	There were no deaths in males or females. Clinical signs of toxicity that were observed included sedation, diarrhea and dyspnea (males). There were no macroscopic changes observed at necropsy.
Conclusions	Under the conditions of this study, Alcohols, C11-14 iso, C13 rich has a low order of acute oral toxicity in rats.
Data Quality	1 - Valid without restrictions
Reference	Research and Consulting Co., (1988). Acute Oral Toxicity Study with Alcohols, C11-14 iso, C13 rich in Rats, Unpublished report.
Date last changed	September, 2000

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Genetic Toxicity

Test Substance CAS No.	1-Dodecanol 112-53-8
Method Type of Study Test system GLP Year Species/Strain	Other Ames Assay <i>S. typhimurium</i> , <i>E. coli</i> Not specified 1985 <i>Salmonella typhimurium</i> /TA98; TA100; TA1535; TA1537; TA1538; <i>E. coli</i> WP2uvrA
Metabolic Activation Concentrations Statistical methods	Yes 0.01, 0.05, 0.1, 0.5, 1, 5, 10, and 50 ug/plate. Samples run in duplicate. No further details provided.
Remarks on Test Conditions	1-dodecanol (90% pure) was dissolved in DMSO at appropriate concentrations. 0.1ml of this mixture was added to 0.1 ml of bacteria and 0.5 ml of either S9 mix (polychlorinated biphenyl-induced rat liver S9 mixture) or phosphate-buffered saline. Following a 20-minute pre-incubation, the mixtures were combined with agar and incubated for 48 hours. Colonies were scored with an automatic counter. All tests were performed in duplicate. 2-(2-Furyl)-3-(5-nitro-2-furyl)acrylamide (AF-2), N-ethyl-N'-nitro-N-nitrosoguanidine (ENNG), 9-aminoacridine (9AC), 4-nitroquinoline-1-oxide (4NQO), benzo(a)pyrene (B(a)P), 2-aminoanthracene (2AA), and 2-nitrofluorene (2NF) were used as positive controls. In addition, water and DMSO were used as vehicle controls.
<u>Results</u>	Negative.
Remarks for Results	There was no evidence of mutagenicity of 1-dodecanol in the presence or absence of metabolic activation in all of the strains tested. The number of revertant colonies per plate did not vary significantly between the water, DMSO, or 1-dodecanol samples.
Conclusions	1-Dodecanol was not mutagenic in bacteria under the conditions of this study.
Data Quality	2- Reliable with restrictions (Similar to OECD 471)
Reference	H. Shimizu, Y. Suzuki, N. Takemura, S. Goto, H. Matsushita, (1985) "The Results of Microbial Mutation Test for Forty-Three Industrial Chemicals," <i>Japanese Journal of Industrial Health</i> , 27 : 400-419.
Date last changed	October 3, 2000

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Repeat Dose Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals Route of administration Frequency of treatment Doses Vehicle</p> <p>Remarks on Test Conditions</p> <p>Results</p> <p>Remarks</p> <p>Conclusions</p>	<p>Alcohols, C11-14 iso, C13 rich 68526-86-3</p> <p>OECD 408 Repeated dose 90-day oral toxicity study Yes 1986 Rats/Sprague-Dawley Males and Females 20/sex/dose Oral gavage Daily, 7 days per week, 14 weeks 0, 100, 500, and 1000 mg/kg/day Distilled water</p> <p>Rats (20/sex/dose) were administered 0, 100, 500, and 1000 mg/kg/day in a dose volume of 10 ml/kg/day for a total period of 14 weeks. Animals were observed daily for signs of toxicity. Body weight was recorded prior to the initial dose, at the initiation of dosing, and weekly thereafter. At the end of the study full serum chemistry and hematology analyses were performed. A full necropsy was performed on each animal and tissues and organs were preserved.</p> <p>NOAEL = 100 mg/kg/day</p> <p>During the study, there were 5 deaths that could not be attributed to treatment with the test substance. Males in the middle and high dose groups had significantly lower body weights and food consumption than the control animals. However, females did not display any differences in body weight or food consumption.</p> <p>Females in the middle and high dose group had statistically significant higher mean platelet counts compared to the control groups. The males did not show any significant differences in mean hematological values. Mean cholesterol increased in high-dose females and glucose decreased in middle-dose females and high-dose animals of both sexes. However, the significance of these findings to treatment with Alcohols, C11-14 iso, C13 rich is not clear.</p> <p>Males and females in the middle and high-dose groups had significantly higher liver weights than animals in the control group. High dose males had significantly lower body weights than the control animals. Relative mean brain and testes weights also increased in high-dose males, while relative adrenal weights increased in high-dose females. However, no treatment-related weight or histopathologic changes were observed in the other organs, including female reproductive organs.</p> <p>Under the conditions of this study, subchronic oral exposure to the lowest concentration (100 mg/kg/day) of Alcohols, C11-14 iso, C13 rich was not toxic. At higher concentrations, there were some effects on hematologic profile and organ weight, but the significance of these changes is not known.</p>
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Data Quality	1 - Valid without restrictions
Reference	Exxon Biomedical Sciences, Inc. (1986); Subchronic oral gavage study in rats; Unpublished report.
Date last changed	October, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No.	Alkenes, C11-13, C12 rich 68526-58-9
Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels:	NA Oral LD ₅₀ Pre-GLP 1961 Rats /Sprague-Dawley Male 5/dose Oral gavage Corn oil Single Treatment Either 0.1, 1.0, and 10.0% volume/volume in corn oil or undiluted. (Equivalent to 24.5, 77.4, 245, 774, 2446, and 7440 mg/kg)
Control group and Treatment:	For comparison, untreated animals were necropsied at the end of the study.
Remarks on Test Conditions	Prior to dosage, food was withheld from the animals for three hours. Following exposure, food and water was available at all times. The animals were observed for gross effects and mortality at 1, 4, and 24 hours and once daily thereafter for 7 days. Gross necropsies were performed at the end of the observation period. Tissue samples from the 2446 and 7440 mg/kg dose levels were collected for possible further analysis.
Results (LD₅₀ or LC₅₀):	LD ₅₀ > 7740 mg/kg
Remarks	No mortalities were observed at any of the doses tested. Animals at all dosage levels exhibited normal appearance and behavior throughout the entire study and showed normal body weight gain. There were no pathological findings at necropsy.
Conclusions	Under the conditions of this study, Alkenes, C11-13, C12-rich have a low order of toxicity.
Data Quality	1 - Reliable without restrictions, comparable to a guideline study
Reference	Hazleton Laboratories, Inc.: Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co., 1961.
Date last changed	October, 2000

Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

<p>Test Substance CAS No.</p> <p>Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:</p> <p>Remarks on Test Conditions</p> <p>Results (LD₅₀ or LC₅₀):</p> <p>Remarks</p> <p>Conclusions</p> <p>Data Quality</p> <p>Reference</p> <p>Date last changed</p>	<p>Alkenes, C11-13, C12 rich 68526-58-9</p> <p>NA Dermal LD₅₀ Pre-GLP 1961 Albino rabbits Males and Females 2/sex/dose Dermal NA Single 24-hour exposure 77.4, 245, 774, 2446 mg/kg. NA</p> <p>Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 7 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. Tissue samples were taken from animals at the 774 and 2446 mg/kg dose levels.</p> <p>LD₅₀ > 2446 mg/kg</p> <p>No mortalities were observed at any dose tested. One animal in the 245 mg/kg dose group had diarrhea on the last day of the study and a net loss of weight. The remaining animals exhibited normal appearance and behavior throughout the entire study and showed normal body weight gain. One animal in the 1000 µl/kg and two animals in the 2446 mg/kg dose groups had parasitic infections in the liver. No other abnormalities were observed at necropsy.</p> <p>Upon removal of the binders, the exposed skin showed slight erythema. Three of the high dose animals displayed slight edema, which subsided within 48 hours. By 48 hours, low dose animals showed no signs of irritation. Erythema in the high dose animals completely subsided by the third day. By Day 12, all signs of irritation had completely cleared in all of the animals with the exception of slight desquamation in one high dose animal.</p> <p>Alkenes, C11-13, C12-rich have a low order of acute dermal toxicity.</p> <p>1 - Reliable without restrictions; comparable to a guideline study.</p> <p>Hazleton Laboratories, Inc.: Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co., 1961.</p> <p>October, 2000</p>
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Robust Summaries - Olefin Hydroformylation Products

Acute Toxicity

Test Substance CAS No. Method/Guideline Type of Study GLP Year Species/strain Sex No. of animals/sex/dose Route of administration Vehicle Frequency of Treatment: Dose/Concentration Levels: Control group and Treatment:	Alkenes, C11-13, C12 rich 68526-58-9 NA Inhalation LC ₅₀ Pre-GLP 1961 Mice/Swiss Albino, Rats/Wistar, Guinea pigs/English short hair Males 10/species Inhalation NA Single Dose 4.4 mg/L for 6 hours (saturated vapors only, no aerosol) Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group.
Remarks on Test Conditions	Air was bubbled through the test material and into a chamber to give a total flow through the chamber of 35 liters/minute. The theoretical mean chamber concentration (4.4 mg/L) was calculated from the loss of material and airflow through the chamber. Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study.
Results (LD₅₀ or LC₅₀):	LC₅₀ > 4.4 mg/L for 6 hours
Remarks	Immediately following initiation of the exposure, all animals exhibited increased motor activity. Lacrimation was observed in rats and guinea pigs beginning at the 90-minute interval. Otherwise, all animals seemed normal in appearance and behavior throughout the study. No abnormalities were observed at necropsy.
Conclusions	Under conditions of this study, Alkenes, C11-13, C12 rich have a low order of acute inhalation toxicity in rats.
Data Quality	2 - Valid with restrictions. No analysis of exposure atmosphere.
Reference	Hazleton Laboratories, Inc.: Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co., 1961.
Date last changed	October, 2000

Attachment II

I U C L I D

Data Set

Existing Chemical	: ID: 104-76-7
CAS No.	: 104-76-7
EINECS Name	: 2-ethylhexan-1-ol
EINECS No.	: 203-234-3
TSCA Name	: 1-Hexanol, 2-ethyl-
Molecular Formula	: C ₈ H ₁₈ O

Producer Related Part	
Company	: EUROPEAN COMMISSION- European Chemicals Bureau
Creation date	: 10.02.2000

Substance Related Part	
Company	: EUROPEAN COMMISSION- European Chemicals Bureau
Creation date	: 10.02.2000

Memo	:
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Printing date	: 05.11.2001
Revision date	: 10.02.2000
Date of last Update	: 10.02.2000

Number of Pages	: 163
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Chapter (profile)	:
Reliability (profile)	:
Flags (profile)	:

1. General Information

Id 104-76-7
Date 05.11.2001

1.0.1 OECD AND COMPANY INFORMATION

Type :
Name : Alusuisse Italia Spa
Partner :
Date :
Street : via del Pruneto, 40
Town : I-52027 S.Giovanni Valdarno (AR)
Country : Italy
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : Alusuisse Italia Spa
Partner :
Date :
Street : via del Pruneto, 40
Town : I-52027 S.Giovanni Valdarno (AR)
Country : Italy
Phone : 055/940032
Telefax : 055/943936
Telex : 570447
Cedex :

Type :
Name : Atochem
Partner :
Date :
Street :
Town : 92080 Paris la Defense
Country : France
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : Atochem
Partner :
Date :
Street : 4, Cours Michelet
Town : 92080 Paris la Defense
Country : France
Phone :
Telefax :

1. General Information

Id 104-76-7
Date 05.11.2001

Telex :
Cedex :

Type :
Name : BASF AG
Partner :
Date :
Street : Karl-Bosch-Str
Town : 67056 Ludwigshafen
Country : Germany
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : BASF AG
Partner :
Date :
Street : Karl-Bosch-Str
Town : 67056 Ludwigshafen
Country : Germany
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : BASF Espanola S. A.
Partner :
Date :
Street :
Town : 43080 Tarragona
Country : Spain
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : BASF Espanola S. A.
Partner :
Date :
Street :
Town : 43080 Tarragona
Country : Spain
Phone :
Telefax :
Telex :
Cedex :

1. General Information

Id 104-76-7
Date 05.11.2001

Type :
Name : BP Chemicals Ltd.
Partner :
Date :
Street : Belgrave House, 76 Buckingham Palace Road
Town : SW1 WOSU London
Country : United Kingdom
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : BP Chemicals Ltd.
Partner :
Date :
Street : 76, Buckingham Palace Road
Town : SW1 WOSU London
Country : United Kingdom
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : BUNA GMBH
Partner :
Date :
Street : Sparte Organica Bau G59
Town : 06258 Schkopau
Country : Germany
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : BUNA GMBH
Partner :
Date :
Street : Sparte Organica Bau G59
Town : 06258 Schkopau
Country : Germany
Phone : 03461 49 2007
Telefax : 03461 49 2670
Telex :
Cedex :

Type :

1. General Information

Id 104-76-7
Date 05.11.2001

Name : Celanese GmbH
Partner :
Date :
Street : Industriepark Höchst
Town : 65926 Frankfurt am Main
Country : Germany
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : Ciba-Geigy SpA
Partner :
Date :
Street : S.S.233 Km 20.5 Varesina
Town : I-21047 Saronno(VA)
Country : Italy
Phone : 39 2 96541
Telefax : 39 2 96701091
Telex :
Cedex :

Type :
Name : CYTEC INDUSTRIES B.V.
Partner :
Date :
Street : P.O.Box 5195 , Botlekweg 175
Town : 3197 ZH Rotterdam
Country : Netherlands
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : ECEM European Chemical Marketing B.V.
Partner :
Date :
Street : Hogehilweg 10
Town : 1101 CC Amsterdam
Country : Netherlands
Phone : 020-6912001
Telefax : 020-6911930
Telex :
Cedex :

Type :
Name : Helm AG
Partner :
Date :
Street : Nordkanalstrasse 28
Town : 20097 Hamburg
Country : Germany
Phone : +49402375-0
Telefax : +49402375-90
Telex : 2170150
Cedex :

Type :
Name : Hoechst AG
Partner :

1. General Information

Id 104-76-7

Date 05.11.2001

Date	:	
Street	:	
Town	:	65903 Frankfurt/Main
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	
Name	:	Hoechst AG
Partner	:	
Date	:	
Street	:	Postfach 80 03 20 Brünigstrasse 50
Town	:	65903 Frankfurt/Main
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Type	:	
Name	:	Huels AG
Partner	:	
Date	:	
Street	:	Postfach
Town	:	45764 Marl
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	
Name	:	Huels AG
Partner	:	
Date	:	
Street	:	Postfach
Town	:	D-45764 Marl
Country	:	Germany
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Type	:	
Name	:	International Speciality Chemicals Ltd.
Partner	:	
Date	:	
Street	:	Charleston Industries Estate, Hardley, Hythe

1. General Information

Id 104-76-7
Date 05.11.2001

Town : SO45 32G Southampton
Country : United Kingdom
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : Lubrizol Great Britain Limited
Partner :
Date :
Street : P.O.Box 88
Town : DE56 1QN Belper, Derby
Country : United Kingdom
Phone : 332-842211
Telefax : 332-842303
Telex : 37445
Cedex :

Type :
Name : Neste Oxo AB
Partner :
Date :
Street :
Town : 444 84 Stenungsund
Country : Sweden
Phone :
Telefax :
Telex :
Cedex :
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Type :
Name : Neste Oxo AB
Partner :
Date :
Street :
Town : 44484 Stenungsund
Country : Sweden
Phone : +46 303 85600
Telefax : +46 303 856 07
Telex : 27052 nestox S
Cedex :

Type :
Name : Petrasol B.V.
Partner :
Date :
Street : P.O.Box 222
Town : 4200 AE Gorinchem
Country : Netherlands
Phone : +31 183 630555
Telefax : +31 183 632272
Telex : 23602 petr nl
Cedex :

Type :

1. General Information

Id 104-76-7
Date 05.11.2001

Name : Vinyl Additives GmbH formerly CIBA Additive GmbH
Partner :
Date :
Street : Chemiestrasse
Town : D-68623 Lampertheim
Country : Germany
Phone : +49(6206)15-0
Telefax : +49(6206)152511
Telex :
Cedex :

Type :
Name : VOSB.V.
Partner :
Date :
Street : Ondernemingsweg 1A
Town : 2404 HM Alphen aan den Rijn
Country : Netherlands
Phone : 31-172-431601
Telefax : 31-172-432494
Telex :
Cedex :

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : inorganic
Physical status : liquid
Purity : % w/w

Substance type : organic
Physical status : liquid
Purity : % w/w

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1-Ethyl-1-hexanol
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1. General Information

Id 104-76-7
Date 05.11.2001

1-Hexanol, 2-ethyl-

Source : Huels AG Marl

1-Hexanol, 2-ethyl- (8Cl, 9Cl)

Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-EH

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethyl-1-hexanol

Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-ethyl-1-hexanol

Remark : Also known as:
2-ethylhexyl alcohol
2-EH
Iso-octanol

Source : International Speciality Chemicals Ltd. Southampton

2-Ethylhexaan-1-ol

Source : VOS B.V. Alphen aan den Rijn

2-Ethylhexanol

Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Huels AG Marl
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Vinyl Additives GmbH formerly CIBA Additive GmbH
Lampertheim

2-Ethylhexanol iso-Octanol

Source : BUNA GMBH Schkopau
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BUNA GMBH Schkopau
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1. General Information

Id 104-76-7
Date 05.11.2001

Celanese GmbH Frankfurt am Main

2-Ethylhexanol-1

Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol; 2-Ethylhexylalcohol; Isooctanol; Octylalcohol; 2-EH

Source : Atochem Paris la Defense
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexanol; ethylhexanol

Source : ISIS/RISKLINE release VI, 1997, Haskoning
Petrasol B.V. Gorinchem

2-Ethylhexyl alcohol

Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Ethylhexylalkohol

Source : Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2-Etil esanolo

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2EH

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)

alcol 2-etilesilico

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)

1. General Information

Id 104-76-7
Date 05.11.2001

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Ethylhexanol
Source

: BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona
Neste Oxo AB Stenungsund
Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Isooctanol
Source

: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

isooctanol
Source

: Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Octyl alcohol
Source

: Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

Production during the last 12 months :
Import during the last 12 months :
Quantity : 500 000 - 1 000 000 tonnes in

1. General Information

Id 104-76-7
Date 05.11.2001

Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Flag : non confidential

Production during the last 12 months :

Import during the last 12 months :

Quantity : more than 1 000 000 tonnes in

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

Type : type
Category : Non dispersive use

Type : type
Category : Use in closed system

Type : type
Category : Wide dispersive use

Type : industrial
Category : Basic industry: basic chemicals

Type : industrial
Category : Chemical industry: used in synthesis

Type : industrial
Category : Paints, lacquers and varnishes industry

Type : industrial
Category : Polymers industry

Type : industrial
Category : Textile processing industry

Type : industrial
Category : other

Type : use
Category : Fuel additives
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Flag : non confidential

Type : use
Category : Fuel additives
Source : ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

1. General Information

Id 104-76-7
Date 05.11.2001

Flag	:	non confidential
Type	:	use
Category	:	Fuel additives
Type	:	use
Category	:	Intermediates
Type	:	use
Category	:	Lubricants and additives
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main
Flag	:	non confidential
Type	:	use
Category	:	Lubricants and additives
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	use
Category	:	Lubricants and additives
Type	:	use
Category	:	Softeners
Source	:	ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Flag	:	non confidential
Type	:	use
Category	:	Softeners
Type	:	use
Category	:	Solvents
Type	:	use
Category	:	other

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit	:	MAK (DE)
Limit value	:	
Remark	:	Kein MAK-Wert festgelegt
Source	:	BASF AG Ludwigshafen BASF Espanola S. A. Tarragona BASF AG Ludwigshafen BASF Espanola S. A. Tarragona ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main BASF AG Ludwigshafen BASF Espanola S. A. Tarragona ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

1. General Information

Id 104-76-7
Date 05.11.2001

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(1)

Type of limit : MAK (DE)
Limit value :
Country : Germany
Remark : MAK not established.
Source : Huels AG Marl

(2)

Type of limit : OES (UK)
Limit value : 271 mg/m3
Short term exposure
Limit value :
Schedule : 8 hour(s)
Frequency : times
Remark : UK OES not assigned specifically. Figure quoted is for Iso-octyl alcohol (mixed isomers) - from EH40 1998 edition.
Source : International Speciality Chemicals Ltd. Southampton

Type of limit : TLV (US)
Limit value : 250 mg/m3
Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark : No data on Occupational Exposure Limit Value.
Source : Atochem Paris la Defense

Remark : No Occupational Exposure Limit available.
Source : Neste Oxo AB Stenungsund

1.9 SOURCE OF EXPOSURE

Remark : PROFESSIONAL/OCCUPATIONAL EXPOSURE DURING PRODUCTION

Process description

1. Production of "oxo alcohols" (2-ethylhexanol, normal and iso-butanol) is performed through several steps of continuous and closed chemical processes.
The first step is the production of synthesis gas obtained by partial oxidation of natural gas.
This so called syngas is used to hydroformylate propylene, a reaction which produces a mixture of n - and isobutyraldehyde.

- 2-Ethylhexanol production
2ethylhexanol is produced by aldolisation of normal butyraldehyde, followed by hydrogenation and distillation.
- Storage and despatch of Oxo Alcohols
Oxo alcohols are stored in closed tanks where vent gas is collected and burnt in a residual gas incinerator.
There is no equipment opening during production, hence exposure to chemicals is quite limited.

exposure to chemicals is quite limited.

Product despatch is done by road, rail, or ship mainly.

2. Number of sites

One production site located in Lavera, France.

3. Protective measures

Procedures and equipment used minimise personnel exposure. Workers and contractors wear gloves, safety glasses or goggles, and long sleeves clothes.

4. Industrial hygiene monitoring

Continuous on line exhalimeters detect leaks.

Local explosivity analysis is made before maintenance work.

Outside operators are watching any abnormal noise or odor.

Routine analysis of hydrocarbon in atmosphere is done.

Worker have a yearly medical follow up.

COV monitoring program underway : will be finished in 18 months.

ENVIRONMENTAL EXPOSURE DURING PRODUCTION AND USE

1. Distribution pattern

Production losses ethyl -2-hexanol

to air 0.001 %

to water 0.004 %

2. Primary exposed environment

All spills are collected. Plant drainage is collected to chemical water sewer. This water is treated in a water treatment plant.

3. Release pattern

Point source and diffuse.

GENERAL USE PATTERN

100 % professional use.

ADDITIONAL INFORMATION

1. Indication of measured exposure levels.

Atmosphere analysis performed 2 times per year indicate an average value of 4 vpm of chemical expressed as CH₄. VOC monitoring program will allow a better follow up.

Source

: Atochem Paris la Defense
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Atochem Paris la Defense
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark

: La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti. Il processo dove viene impiegata la sostanza è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Purificazione
- Filtrazione

Tutte le fasi del processo vengono condotte a ciclo chiuso

Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe, tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.

Gli effluenti del processo sono i seguenti:

- 1) Acqua di reazione
- 2) Gas incondensabili

L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto ecologico dello Stabilimento, quindi immessa in acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).

Dati relativi alle emissioni

Acque trattate :

- * tipo di emissione - puntiforme
- * Durata emissione - continua

Emissioni atmosfera:

- * tipo di emissione - puntiforme
- * Portata - 25 Nm³/h per Ton. di sostanza
- * durata emissione - continua

Fattori potenziali di esposizione umana

La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresì una buona soglia olfattiva. Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source

: Alusuisse Italia Spa S.Giovanni Valdarno (AR)

Country Remark

: Sweden

: One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

Source	: No 2-ethylhexanol is used in consumer products. Neste Oxo AB Stenungsund	(3)
Remark	<p>: La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti. Il processo dove viene impiegata la sostanza è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:</p> <ul style="list-style-type: none">- Reazione- Purificazione- Filtrazione <p>Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe , tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso. Gli effluenti del processo sono i seguenti: 1) Acqua di reazione 2) Gas incondensabili</p> <p>L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto ecologico dello Stabilimento, quindi immessa in acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).</p> <p>I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).</p> <p>Dati relativi alle emissioni</p> <p>Acque trattate :</p> <ul style="list-style-type: none">* tipo di emissione - puntiforme* Durata emissione - continua <p>Emissioni atmosfera:</p> <ul style="list-style-type: none">* tipo di emissione - puntiforme* Portata - 25 Nm3/h per Ton. di sostanza* durata emissione - continua <p>Fattori potenziali di esposizione umana La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresì una buona soglia olfattiva. Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.</p> <p>Settori di impiego</p> <p>La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la</p>	

1. General Information

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plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Country : Sweden

Remark : One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

No 2-ethylhexanol is used in consumer products.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(3)

Remark : La sostanza in esame è utilizzata come materia prima nello Stabilimento Distillerie Italiane dell'Alusuisse Italia Spa, nel processo di sintesi dei plastificanti.
Il processo dove viene impiegata la sostanza è di tipo discontinuo (per batch) e consiste essenzialmente nelle seguenti fasi:

- Reazione
- Purificazione
- Filtrazione

Tutte le fasi del processo vengono condotte a ciclo chiuso in quanto tutte le sostanze coinvolte nella sintesi chimica sono movimentate attraverso pompe, tubazioni, sistemi di trasferimento e apparecchiature di tipo chiuso.

Gli effluenti del processo sono i seguenti:

- 1) Acqua di reazione
- 2) Gas incondensabili

L'acqua di reazione, contenente tracce di sostanze organiche, viene raccolta e trasferita al trattamento di depurazione nell'impianto ecologico dello Stabilimento, quindi immessa in acque superficiali nei limiti stabiliti dalle leggi nazionali (Legge Merli n° 319/76).

I gas ricondensabili, contenenti tracce di sostanze organiche, provenienti dalle apparecchiature di processo, sono collettati e inviati al trattamento di depurazione in apposito impianto di ossidazione termica e quindi immessi in atmosfera in conformità alle leggi nazionali vigenti (DPR 203/88).

Dati relativi alle emissioni

Acque trattate :

- * tipo di emissione - puntiforme
- * Durata emissione - continua

* Durata emissione - continua

Emissioni atmosfera:

- * tipo di emissione - puntiforme
- * Portata - 25 Nm³/h per Ton. di sostanza
- * durata emissione - continua

Fattori potenziali di esposizione umana
La sostanza ha un'alta temperatura di ebollizione ed una bassa tensione di vapore, presenta altresì una buona soglia olfattiva. Considerando che la sostanza viene utilizzata in processi a ciclo chiuso si ritiene insignificante il potenziale di esposizione ai vapori da parte dell'utilizzatore.

Settori di impiego

La sostanza fa parte della famiglia degli OXOalcoli e viene impiegata come materia prima nel processo di sintesi del plastificante che a sua volta costituisce un additivo per la produzione di materiali termoplastici a base di PVC. Nel plastificante la sostanza non si trova più allo stato libero ma come estere dell'anidride ftalica.

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Country : Sweden
Remark : One plant in Sweden produces 2-ethylhexanol. The production units are located outdoors and the average concentration in the air is 0.02 ppm. The type of release to the air is both point source and diffuse.

The major part of produced 2-ethylhexanol is used in the production of plasticisers.

The production of 2-ethylhexanol is a closed process.

Source : No 2-ethylhexanol is used in consumer products.
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(3)

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 2 (water polluting)
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

Classified by : KBwS (DE)
Labelled by :
Class of danger : 2 (water polluting)
Country : Germany
Remark : Kenn-Nr. 134
Source : Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Huels AG Marl
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(4)

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 2 (water polluting)
Country : Germany
Remark : Katalognummer 134
Source : Huels AG Marl

(2)

1.14.2 MAJOR ACCIDENT HAZARDS

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Source : BASF AG Ludwigshafen
BASF Espanola S. A. Tarragona

(5)

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Source : Hoechst AG Frankfurt/Main

(6)

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Country : Germany
Remark : Stoerfallverordnung 1991
Source : Huels AG Marl

(2)

Legislation : Stoerfallverordnung (DE)
Substance listed : no

1. General Information

Id 104-76-7
Date 05.11.2001

No. in directive :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(6)

1.14.3 AIR POLLUTION

Classified by : TA-Luft (DE)
Labelled by : TA-Luft (DE)
Number : 3.1.7 (organic substances)
Class of danger : III
Source : BASF Espanola S. A. Tarragona

(7)

Classified by : TA-Luft (DE)
Labelled by :
Number : 3.1.7 (organic substances)
Class of danger : III
Remark : Selbsteinstufung
Source : Hoechst AG Frankfurt/Main

(8)

Classified by : TA-Luft (DE)
Labelled by : TA-Luft (DE)
Number : 3.1.7 (organic substances)
Class of danger : III
Country : Germany
Remark : Appendix E
Source : Huels AG Marl

(2)

Classified by : TA-Luft (DE)
Labelled by :
Number : 3.1.7 (organic substances)
Class of danger : III
Remark : Selbsteinstufung
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

1.15 ADDITIONAL REMARKS

Remark : Possibilità di eliminazione

La sostanza ha una bassa solubilità in acqua (ca 0.1 mg/l);
può essere eliminata per ossidazione biologica in appositi
impianti di trattamento.

La sostanza può essere eliminata anche per ossidazione
termica in appositi impianti di incenerimento con recupero
energetico e controllo emissioni all'atmosfera secondo la
normativa vigente.

Informazioni relative al trasporto

La sostanza che viene importata ed utilizzata come materia
prima viaggia su carri cisterna ferroviari secondo la
normativa Internazionale RID appartenendo alla classe 3
ordinale 32° c), indice KEMLER e n° ONU 30/1987.

1. General Information

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Tipo del numero: ferrocisterna per prodotti RID

Quantità media
trasportata : 56.000 kg

Ferrocisterne/mese: 4

Misure di controllo
durante il trasporto: Il prodotto viaggia con la
documentazione stabilita dalle
leggi vigenti in materia
(normativa RID)

Source : Alusuisse Italia Spa S.Giovanni Valdarno (AR)
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Alusuisse Italia Spa S.Giovanni Valdarno (AR)
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Remark : Wasserschadstoffklasse 2
Source : BUNA GMBH Schkopau

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

2.1 MELTING POINT

Value : -76 - 70 ° C
Source : Neste Oxo AB Stenungsund (10)

Value : -76 - 70 ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (11)

Value : -76 - 70 ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (11)

Value : < -60 ° C
Sublimation :
Method : other: DIN 3016
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund (12)

Value : < -60 ° C
Sublimation :
Method : other: DIN 3016
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main (8)

Value : < -60 ° C
Sublimation :
Method : other: DIN 3016
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

2.2 BOILING POINT

Value : = 184.5 ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

Value : = 184.5 ° C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

(9)

Value : = 184.5 °C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 °C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 °C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 184.5 °C at 1013 hPa
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

2.3 DENSITY

Type : density
Value : = .83 g/cm³ at 20° C
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(11)

Type :
Value : ca. .832 - .833 at 20° C
Source : ECEM European Chemical Marketing B.V. Amsterdam

Type : density
Value : = .832 g/cm³ at 20° C
Method : other: DIN 51757
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

(13)

Type : density
Value : = .832 g/cm³ at 20° C
Method : other: DIN 51757
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main

(8)

Type : density
Value : = .832 g/cm³ at 20° C

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

Method : other: DIN 51757
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Type : density
Value : = .84 g/cm³ at 20° C
Source : BASF AG Ludwigshafen

(14)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .05 at 20° C
Source : ECEM European Chemical Marketing B.V. Amsterdam

Value : .144 hPa at 20° C
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(15)

Value : = .144 hPa at 20° C
Source : BASF AG Ludwigshafen

(15)

Value : .4 hPa at 20° C
Decomposition :
Method : other (calculated): calculated
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

(13)

Value : = .4 hPa at 20° C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main

(8)

Value : = .4 hPa at 20° C
Decomposition :
Method : other (calculated)
Year :
GLP :

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

Value : ca. .13 hPa at 25° C
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (16)

Value : 2.9 hPa at 50° C
Decomposition :
Method : other (calculated): calculated
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund (13)

Value : = 2.9 hPa at 50° C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main (8)

Value : = 2.9 hPa at 50° C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

2.5 PARTITION COEFFICIENT

Log pow : = 2.28 at ° C
Method : other (calculated): calculated; Leo and Hansch
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund (13)

Log pow : = 2.28 at ° C
Method : other (calculated): Leo und Hansch
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

(8)

Log pow : = 2.28 at ° C
Method : other (calculated): Leo und Hansch
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Log pow : 2.809 at ° C
Method : other (calculated)
Year :
GLP :
Test substance :
Remark : Calculated according to Leo and Hansch, MedChem-Programm, Version 1989 (POMONA89)
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Log pow : ca. 3 at ° C
Source : BASF AG Ludwigshafen

(17)

Log pow : = 3.1 at ° C
Method : OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year : 1981
GLP : no data
Test substance :
Source : Neste Oxo AB Stenungsund

(18)

Log pow : = 3.1 at ° C
Method : OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year : 1981
GLP : no data
Test substance :
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(19)

Log pow : = 3.1 at ° C
Method : OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year : 1981
GLP : no data
Test substance :
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(19)

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

2.6.1 WATER SOLUBILITY

Value : = .1 at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : ECEM European Chemical Marketing B.V. Amsterdam

Value : ca. 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : Neste Oxo AB Stenungsund

(14)

Value : = 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : = 7 at 1 g/l and 20 ° C
Source : Neste Oxo AB Stenungsund

(13)

Value : ca. 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : BASF AG Ludwigshafen

(15)

Value : = 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : = 7 at 1 g/l and 20 ° C
Source : Hoechst AG Frankfurt/Main

(8)

Value : ca. 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(15)

Value : = 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : = 7 at 1 g/l and 20 ° C
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : ca. 1 g/l at 20 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(15)

Value : = 1100 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(20)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : = 73 ° C
Type : closed cup
Source : ECEM European Chemical Marketing B.V. Amsterdam

Value : = 75 ° C
Type :
Method : other: DIN 51758
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

(13)

Value : = 75 ° C
Type :
Method : other: DIN EN 22719, ISO 2719
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main

(8)

Value : = 75 ° C
Type :
Method : other: DIN EN 22719, ISO 2719
Year :
GLP :
Test substance :
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(9)

Value : = 76 ° C
Type :
Method : other: DIN 51 758
Year :

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (15)

Value : = 82 ° C
Type : closed cup
Method : other
Year :
GLP :
Test substance :
Remark : Method: DIN 51758
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (21)

2.8 AUTO FLAMMABILITY

Value : = 270 ° C at
Method : other: DIN 51 794
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
BASF AG Ludwigshafen
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (15)

Value : = 305 ° C at
Method : other: DIN 51794
Year :
GLP :
Test substance :
Remark : Auto-ignition temperature
Source : Neste Oxo AB Stenungsund (13)

Value : = 305 ° C at
Method : other: DIN 51794
Year :

2. Physico-Chemical Data

Id 104-76-7
Date 05.11.2001

GLP :
Test substance :
Remark : Zuendtemperatur
Source : Hoechst AG Frankfurt/Main (8)

Value : = 305 ° C at
Method : other: DIN 51794
Year :
GLP :
Test substance :
Remark : Zuendtemperatur
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

Value : 330 ° C at
Method : other
Year :
GLP :
Test substance :
Remark : Method: DIN 51794
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (19)

2.9 FLAMMABILITY

Result : other: when heated vapors may form explosive mixtures with air
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

2.10 EXPLOSIVE PROPERTIES

Result : other
Remark : Explosionsgrenze: 1.1 - 12.7 Vol.-%
Source : Hoechst AG Frankfurt/Main (8)

Result : other
Remark : Explosionsgrenze : 1.1 - 12.7 Vol.-%
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

Result : other: Explosionsgrenzen 1.1 - 7.4 Vol.%

2. Physico-Chemical Data

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Date 05.11.2001

Source : BASF AG Ludwigshafen (14)

Remark : Explosive limits in air: 1.1 -12.7 vol-%
Source : Neste Oxo AB Stenungsund (13)

2.11 OXIDIZING PROPERTIES

Source : Neste Oxo AB Stenungsund

2.12 ADDITIONAL REMARKS

Remark : Remark 1: Viscosity
12 mm²/s at 20 degrees C
35 mm²/s at 0 degrees C
Remark 2: Henry's law constant: 2.65 E-5 atm x m³ x mole⁻¹
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (22) (23)

Remark : Dynamic viscosity: 10 mPas at 20 degrees C.
(Method: DIN 51562)
Source : Neste Oxo AB Stenungsund (13)

Remark : Viskosität: 8.8 mPa.s (20 Grad C)
Source : BASF AG Ludwigshafen (14)

Remark : Dynamische Viskosität bei 20 Grad C: 10 mPas
(Methode: DIN 51562)
Source : Hoechst AG Frankfurt/Main (8)

Remark : Dynamische Viskosität bei 20 Grad C: 10 mPas
(Methode: DIN 51562)
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

Remark : Gefährliche Reaktionen: mit Oxidationsmitteln
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (9)

3. Environmental Fate and Pathways

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3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spect. : nm
Rel. intensity : based on Intensity of Sunlight
Indirect photolysis
Sensitizer : OH
Conc. of sens. : 1500000 molecule/cm3
Rate constant : = .00000000001296 cm3/(molecule*sec)
Degradation : ca. 50 % after 9.9 hour(s)
Deg. Product :
Method : other (calculated): calculated; AOPWIN, Version 1.55, April 1994, Syracuse Research
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : No study located.
Source : Neste Oxo AB Stenungsund

Type : air
Light source :
Light spect. : nm
Rel. intensity : based on Intensity of Sunlight
Indirect photolysis
Sensitizer : OH
Conc. of sens. : 1500000 molecule/cm3
Rate constant : = .00000000001296 cm3/(molecule*sec)
Degradation : ca. 50 % after 9.9 hour(s)
Deg. Product :
Method : other (calculated): AOPWIN, Version 1.55, April 1994, Syracuse Research
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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3.1.2 STABILITY IN WATER

Remark : Study not located.
Source : Neste Oxo AB Stenungsund

3.1.3 STABILITY IN SOIL

Remark : Koc = 105 (calculated by equation 4-5 in Lyman, et al (1981).
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3. Environmental Fate and Pathways

Id 104-76-7
Date 05.11.2001

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3.2 MONITORING DATA

Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Result : 66-111 ug/l in Hayashida river, Japan.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(26)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Result : 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source : Neste Oxo AB Stenungsund

(27)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Remark : 2-Ethylhexanol detected in Mersey estuary 1990.
Source : Neste Oxo AB Stenungsund

(28)

Type of measurement : background concentration
Medium : drinking water
Method :
Concentration :
Remark : 2-Ethylhexanol detected in "tap water", Japan 1980.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(29)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Result : 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(27)

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Id 104-76-7
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Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Remark : 2-Ethylhexanol detected in Mersey estuary 1990.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
(28)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Result : 3.0-5.0 ug/l in Delaware river (winter), USA, 1977.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(27)

Type of measurement : background concentration
Medium : surface water
Method :
Concentration :
Remark : 2-Ethylhexanol detected in Mersey estuary 1990.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(28)

Type of measurement :
Medium : surface water
Method :
Concentration :
Result : Saskatchewan River, 8 and 20 km downstream from Nipawin,
2-ethylhexanol detected, not quantified.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(30)

Type of measurement :
Medium : surface water
Method :
Concentration :
Result : West Valley, New York: 3.6-8.1 mg/l
Source : Neste Oxo AB Stenungsund
(31)

Type of measurement :
Medium : surface water
Method :
Concentration :
Result : West Valley, New York: 3.6-8.1 mg/l
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)

3. Environmental Fate and Pathways

Id 104-76-7
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(31)

Type of measurement :
Medium : surface water
Method :
Concentration :
Result : West Valley, New York: 3.6-8.1 mg/l
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(31)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Remark : No study located.
Source : Neste Oxo AB Stenungsund

3.3.2 DISTRIBUTION

Media : other
Method : Calculation according Mackay, Level I
Year :
Remark : Media: air-water-sediment-soil.

Source : Result: air 16%, water 53%, sediment 25%, soil 5.4
Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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3.4 MODE OF DEGRADATION IN ACTUAL USE

Remark : Biological degradation is expected to be the main mode of degradation.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted

3. Environmental Fate and Pathways

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Date 05.11.2001

Concentration : 3.16mg/l related to DOC (Dissolved Organic Carbon)
related to
Contact time :
Degradation : = 55 % after 17 day
Result :
Deg. Product :
Method : Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : The test was performed on the sodium salt, which immediately
dissociates to form the alcohol under the test conditions.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(33)

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 6.32mg/l related to DOC (Dissolved Organic Carbon)
related to
Contact time :
Degradation : = 68 % after 17 day
Result :
Deg. Product :
Method : Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : The test was performed on the sodium salt, which immediately
dissociates to form the alcohol under the test conditions.
Source : Neste Oxo AB Stenungsund

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 6.32mg/l related to DOC (Dissolved Organic Carbon)
related to
Contact time :
Degradation : = 68 % after 17 day
Result :
Deg. Product :
Method : Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : The test was performed on the sodium salt, which immediately
dissociates to form the alcohol under the test conditions.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(33)

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 6.32mg/l related to DOC (Dissolved Organic Carbon)
related to
Contact time :

3. Environmental Fate and Pathways

Id 104-76-7

Date 05.11.2001

Degradation : = 68 % after 17 day
Result :
Deg. Product :
Method : Directive 84/449/EEC, C.5 "Biotic degradation - modified Sturm test"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : The test was performed on the sodium salt, which immediately dissociates to form the alcohol under the test conditions.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(33)

Type : aerobic
Inoculum : activated sludge, domestic
Concentration : 250mg/l related to related to
Contact time :
Degradation : = 100 % after 5 day
Result : inherently biodegradable
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1985
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(34)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Contact time :
Degradation : > 95 % after 5 day
Result :
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1980
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Non-biological elimination: 20-30%
Source : Neste Oxo AB Stenungsund

(35)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Contact time :
Degradation : > 95 % after 5 day
Result :
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1980

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GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Eliminierung durch nicht biol. Vorgänge 20 - 30 %
Source : Hoechst AG Frankfurt/Main

(36)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Contact time :
Degradation : > 95 % after 5 day
Result :
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1980
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Eliminierung durch nicht biol. Vorgänge 20 - 30 %
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(36)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 249mg/l related to Test substance
related to
Contact time :
Degradation : = 97 % after 7 day
Result :
Kinetic of test substance : 1 day = 23 %
2 day = 36 %
5 day = 96 %
7 day = 97 %
%
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 249mg/l related to Test substance
related to
Contact time :
Degradation : = 97 % after 7 day
Result :
Kinetic of test substance : 1 day = 23 %
2 day = 36 %
5 day = 96 %
7 day = 97 %
%
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4

3. Environmental Fate and Pathways

Id 104-76-7
Date 05.11.2001

Source : Hoechst AG Frankfurt/Main (37)

Type : aerobic
Inoculum : activated sludge, industrial, non-adapted
Concentration : 249mg/l related to Test substance related to
Contact time :
Degradation : = 97 % after 7 day
Result :
Kinetic of test substance : 1 day = 23 %
2 day = 36 %
5 day = 96 %
7 day = 97 %
%
Deg. Product :
Method : OECD Guide-line 302 B "Inherent biodegradability: Modified Zahn-Wellens Test"
Year : 1979
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(37)

Type : aerobic
Inoculum : activated sludge, domestic
Concentration : 83mg/l related to Test substance related to
Contact time :
Degradation : = 88 % after 17 day
Result :
Deg. Product :
Method : other: EEC Directive 79-831 Annex V Part C
Year : 1984
GLP :
Test substance :
Remark : Degradation is the measured BOD as percent of ThOD.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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Type : aerobic
Inoculum : other: Belebtschlamm einer kommunalen Kllaeranlage
Concentration : 83mg/l related to Test substance related to
Contact time :
Degradation : = 88 % after 17 day
Result :
Deg. Product :
Method : other: EEC Directive 79-831 Annex V Part C: Methods for the determination of ecotoxicity. Degradation - Biotic Degradation. Manometric Respirometry
Year : 1984
GLP :

3. Environmental Fate and Pathways

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Test substance	:		
Remark	:	Der Abbauwert ist der gemessene biochemische Sauerstoffbedarf BSB als Prozentwert des theoretischen Sauerstoffbedarfs (ThSB).	
Source	:	BASF AG Ludwigshafen	(39)
Type	:	aerobic	
Inoculum	:	activated sludge, non-adapted	
Remark	:	Method: BOD5-20 fresh and sea water.	
		Results: Fresh water Sea water	
		BOD5=26% BOD5=58%	
		BOD10=75% BOD10=64%	
		BOD15=78% BOD15=84%	
		BOD20=86% BOD20=100%	
Source	:	Neste Oxo AB Stenungsund	(40)
Type	:	aerobic	
Inoculum	:	activated sludge, non-adapted	
Remark	:	Method: BOD5-20 fresh and sea water.	
		Results: Fresh water Sea water	
		BOD5=26% BOD5=58%	
		BOD10=75% BOD10=64%	
		BOD15=78% BOD15=84%	
		BOD20=86% BOD20=100%	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(41)
Type	:	aerobic	
Inoculum	:	activated sludge, non-adapted	
Remark	:	Method: BOD5-20 fresh and sea water.	
		Results: Fresh water Sea water	
		BOD5=26% BOD5=58%	
		BOD10=75% BOD10=64%	
		BOD15=78% BOD15=84%	
		BOD20=86% BOD20=100%	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(41)
Type	:	aerobic	
Inoculum	:	aerobic microorganisms	
Concentration	:	.1mg/l related to related to	
Remark	:	Test medium: pure bacteria culture suspension isolated from activated sludge.	
		Results: Normal sewage (domestic waste water) 0% degraded after 24 h. 100% degraded after 5.6 days.	
		Adapted sewage (industrial effluent)	

3. Environmental Fate and Pathways

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Adapted sewage (industrial effluent)
100% degraded after 24h.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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Type : aerobic
Inoculum :
Source : Neste Oxo AB Stenungsund

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Type : aerobic
Inoculum :
Result : Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results: Municipal Industrial

BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

Type : aerobic
Inoculum :
Result : Method: Secondary effluent from municipal and industrial waste water treatment plants was used as seed (25-55 ml/l).

Results: Municipal Industrial

BOD5/COD	0.70	0.60
BOD10/COD	0.81	0.77
BOD20/COD	0.87	0.86

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF : ca. 27
Elimination :
Method : other: Calculation based on water solubility
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund

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BCF : ca. 27
Elimination :
Method : other: Calculation based on water solubility
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

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BCF : ca. 27
Elimination :
Method : other: Calculation based on water solubility
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : flow through
Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 43 hour(s)
Unit : mg/l
Analytical monitoring : no
LC0 : 96 - 144
Method : other: dietary exposure
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Result : No effect on mortality
Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

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Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC50 : 27 - 29.5
Method : other: in Anlehnung an EPA-Guideline
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(47)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no data
NOEC : = 10
LC50 : 29.7
Method : other: keine Angaben
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

4. Ecotoxicity

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Date 05.11.2001

(45)

Type : other
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 5 day
Unit : mg/l
Analytical monitoring : no data
LC50 : = 24
Method : other: keine Angaben
Year :
GLP : no data
Test substance : no data
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test condition : Species: fry, 0.15 g

Test condition: 15 degrees C, pH=7

(48)

Type : other
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no data
LC50 : > 7.5
Method : other: keine Angaben
Year :
GLP : no data
Test substance : no data
Remark : Fry, 0.15 g
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
Test condition : 20 degrees C; pH = 7

(48)

Type : flow through
Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 43 hour(s)
Unit : mg/l
Analytical monitoring :
LC0 : 96 - 144
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Method: dietary exposure.

Result: No effect on mortality.
Source : Neste Oxo AB Stenungsund

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4. Ecotoxicity

Id 104-76-7
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Type : flow through
Species : Leuciscus idus melanotus (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
NOEC : = 14
LC50 : = 17.1
LC100 : = 21
Method : Directive 84/449/EEC, C.1 "Acute toxicity for fish"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(49)

Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
LC50 : 27 - 29.5
Method : other
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund

(47)

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
NOEC : = 10
LC50 : 29.7
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund

(45)

Type : static
Species : Salmo gairdneri (Fish, estuary, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC50 : 32 - 37
Method : other: Range finding acute toxicity test.
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

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Date 05.11.2001

Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(50)

Type : other
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 5 day
Unit : mg/l
Analytical monitoring :
LC50 : = 24
Source : Neste Oxo AB Stenungsund
Test condition : Species: fry, 0.15 g

Test condition: 15 degrees C, pH=7

(51)

Type : other
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
LC50 : > 7.5
Remark : Fry, 0.15 g
Source : Neste Oxo AB Stenungsund
Test condition : 20 degrees C; pH = 7

(48)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no
EC50 : 39
Method : Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(19)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no
EC50 : 39
Method : Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

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Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(19)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no data
EC50 : = 44
Method : OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(45)

Type :
Species : Artemia salina (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no data
EC50 : = 19
Method : other: keine Angaben
Year :
GLP : no data
Test substance : no data
Remark : Species: seawater
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(41)

Type :
Species : Artemia salina (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring :
EC50 : = 19
Remark : Species: seawater
Source : Neste Oxo AB Stenungsund

(41)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no
EC50 : 39
Method : Directive 84/449/EEC, C.2 "Acute toxicity for Daphnia"
Year : 1984
GLP : yes

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Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund (52)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring :
EC50 : = 44
Method : OECD Guide-line 202, part 1 "Daphnia sp., Acute Immobilisation Test"
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund (53)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no
EC50 : = 26
Method : other: Screening test
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (54)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Chlorella emersonii (Algae)
Endpoint : growth rate
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no data
NOEC : = 10
EC50 : 10 - 50
Method : other: keine Angaben
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Method: 22 degrees C, air was passed through the culture.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (48)

4. Ecotoxicity

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Date 05.11.2001

Species : Chlorella emersonii (Algae)
Endpoint : growth rate
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no data
NOEC : = 10
EC50 : 10 - 50
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Method: 22 degrees C, air was passed through the culture.
Source : Neste Oxo AB Stenungsund

(55)

Species : Scenedesmus subspicatus (Algae)
Endpoint : growth rate
Exposure period : 72 hour(s)
Unit : mg/l
Analytical monitoring : yes
NOEC : =
EC10 : = 3.2
EC50 : = 11.5
EC90 : ca. 41.1
Method : Directive 87/302/EEC, part C, p. 89 "Algal inhibition test"
Year : 1988
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(56)

Species : Scenedesmus subspicatus (Algae)
Endpoint : growth rate
Exposure period : 72 hour(s)
Unit : mg/l
Analytical monitoring : no
EC10 : = 1.3
EC50 : = 13.3
EC90 : = 138.5
Method : other: Algal growth inhibition test, UBA
Year : 1984
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
 Species : Pseudomonas putida (Bacteria)
 Exposure period : 18 hour(s)
 Unit : mg/l
 Analytical monitoring : no
 EC10 : = 540
 Method : other: DIN 38412 Part 8
 Year :
 GLP : no
 Test substance : as prescribed by 1.1 - 1.4
 Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main

(19)

Type : aquatic
 Species : Pseudomonas putida (Bacteria)
 Exposure period : 18 hour(s)
 Unit : mg/l
 Analytical monitoring : no
 EC10 : = 540
 Method : other: DIN 38412 Part 8
 Year :
 GLP : no
 Test substance : as prescribed by 1.1 - 1.4
 Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(19)

Type : aquatic
 Species : activated sludge, domestic
 Exposure period : 24 hour(s)
 Unit : mg/l
 Analytical monitoring : no
 SG : ca. 300
 Method : ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
 Year : 1980
 GLP : no
 Test substance : as prescribed by 1.1 - 1.4
 Remark : SG = Schädlichkeitsgrenze
 Source : Hoechst AG Frankfurt/Main
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(36)

Type : aquatic
 Species : activated sludge, domestic
 Exposure period : 24 hour(s)
 Unit : mg/l
 Analytical monitoring :
 SG : ca. 300
 Method : ETAD Fermentation tube method "Determination of damage to effluent bacteria by the Fermentation Tube Method"
 Year : 1980
 GLP : no
 Test substance : as prescribed by 1.1 - 1.4

4. Ecotoxicity

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Remark : SG= Schädlichkeitgrenze
Source : Neste Oxo AB Stenungsund (35)

Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 18 hour(s)
Unit : mg/l
Analytical monitoring : no
EC10 : = 540
Method : other: DIN 38412 Part 8
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund (58)

4.5.1 CHRONIC TOXICITY TO FISH

Remark : Study not located.
Source : Neste Oxo AB Stenungsund

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Remark : Study not located.
Source : Neste Oxo AB Stenungsund

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

Remark : No study located.
Source : Neste Oxo AB Stenungsund

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Remark : Study not located.
Source : Neste Oxo AB Stenungsund

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

Remark : No study located.
Source : Neste Oxo AB Stenungsund

4.7 BIOLOGICAL EFFECTS MONITORING

Remark : Study not located.
Source : Neste Oxo AB Stenungsund

4.8 BIOTRANSFORMATION AND KINETICS

Remark : Study not located.
Source : Neste Oxo AB Stenungsund

4. Ecotoxicity

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4.9 ADDITIONAL REMARKS

5. Toxicity

Id 104-76-7
Date 05.11.2001

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3730 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: 99.5%
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(59)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : 1516 - 2774 mg/kg bw
Method :
Year :
GLP :
Test substance : no data
Source : Neste Oxo AB Stenungsund

(60)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : 3870 - 5520 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: technical grade
Remark : 2-Ethylhexanol (technical grade) was administered to a total of 70 female rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5. Toxicity

Id 104-76-7
Date 05.11.2001

(61)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3700
Method :
Year :
GLP : no
Test substance : no data
Remark : Range of values: 3.61-5.52 ml/kg (3.0-4.6 g/kg)
2-Ethylhexanol was given undiluted; no further details
reported.
Source : Neste Oxo AB Stenungsund

(62)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 7000 mg/kg bw
Method :
Year :
GLP : no
Test substance : no data
Remark : Result: 49 male albino rats (strain not reported) received
single doses of 2-ethylhexanol by gavage at levels of 5, 6,
8, 10, 12, and 15 g/kg bw. Gross necropsy evaluation
revealed congestion of the spleen and liver as well as
paleness of the kidney.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(63)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : 1516 - 2774 mg/kg bw
Method :
Year :
GLP :
Test substance : no data
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(64)

Type : LD50

5. Toxicity

Id 104-76-7
Date 05.11.2001

Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3700
Method :
Year :
GLP : no
Test substance : no data
Remark : Range of values: 3.61-5.52 ml/kg (3.0 -4.6 g/kg)
2-Ethylhexanol was given undiluted; no further details
reported.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(65)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : 1516 - 2774 mg/kg bw
Method :
Year :
GLP :
Test substance : no data
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3700
Method :
Year :
GLP : no
Test substance : no data
Remark : Range of values: 3.61-5.52 ml/kg (3.0 -4.6 g/kg)
2-Ethylhexanol was given undiluted; no further details
reported.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(65)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3768 mg/kg bw

5. Toxicity

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Date 05.11.2001

Method :
Year :
GLP :
Test substance : no data
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(66)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 3280 - 4460 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source : Neste Oxo AB Stenungsund

(67)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 2870 - 3610 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 female mice.
Source : Neste Oxo AB Stenungsund

(68)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3580 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : Range of values: 2900-4420 mg/kg

2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice. The LD50 was calculated 2 days after the test substance administration (no further details reported).

5. Toxicity

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Date 05.11.2001

(no further details reported).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 2500 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : Range of values: 2090-3010 mg/kg.
2-Ethylhexanol (technical grade, undiluted) was administered
to a total of 70 female mice. The LD50 was calculated 1 day
after the test substance administration (no further details
reported).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 3280 - 4460 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in
peanut oil and administered to a total of 70 male mice.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 2870 - 3610 mg/kg bw

5. Toxicity

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Date 05.11.2001

Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 3280 - 4460 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 70 male mice.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : 2870 - 3610 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : Result: 2-Ethylhexanol (technical grade) was diluted 1:3 in peanut oil and administered to a total of 50 femal mice.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(61)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1470 mg/kg bw
Source : Neste Oxo AB Stenungsund

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Type : LD50
Species : rabbit
Strain :

5. Toxicity

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Date 05.11.2001

Sex :
 Number of animals :
 Vehicle :
 Value : = 1180 mg/kg bw
 Method :
 Year :
 GLP : no
 Test substance :
 Remark : 2-Ethylhexanol (technical grade, undiluted) was administered to a total of 12 male rabbits. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(61)

Type : LD50
 Species : rabbit
 Strain :
 Sex :
 Number of animals :
 Vehicle :
 Value : = 1470 mg/kg bw
 Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main

(65)

Type : LD50
 Species : rabbit
 Strain :
 Sex :
 Number of animals :
 Vehicle :
 Value : = 1470 mg/kg bw
 Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(65)

Type : LD50
 Species : guinea pig
 Strain :
 Sex :
 Number of animals :
 Vehicle :
 Value : = 600 mg/kg bw
 Method :
 Year :
 GLP :
 Test substance : as prescribed by 1.1 - 1.4
 Remark : Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.

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Source	: paleness of the kidney. Neste Oxo AB Stenungsund	(70)
Type	: LD50	
Species	: guinea pig	
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	: 1220 - 2820 mg/kg bw	
Method	:	
Year	:	
GLP	:	
Test substance	: other TS: 2-EH technical grade	
Remark	: 2-Ethylhexanol (technical grade) was administered to a total of 12 male guinea pigs. The LD50 was calculated 1 day after the test substance administration.	
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(61)
Type	: LD50	
Species	: guinea pig	
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	: = 600 mg/kg bw	
Method	:	
Year	:	
GLP	: no	
Test substance	:	
Remark	: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.	
Source	: Neste Oxo AB Stenungsund	(71)
Type	: LD50	
Species	: guinea pig	
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Value	: = 600 mg/kg bw	
Method	:	
Year	:	
GLP	:	
Test substance	: as prescribed by 1.1 - 1.4	
Remark	: Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.	

5. Toxicity

Id 104-76-7

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Source : paleness of the kidney.
: Neste Oxo AB Stenungsund
: ECB - Existing Chemicals Ispra (VA)
: Hoechst AG Frankfurt/Main
(63)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.

Source : Neste Oxo AB Stenungsund
: ECB - Existing Chemicals Ispra (VA)
: Hoechst AG Frankfurt/Main
(63)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Result: 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.

Source : Neste Oxo AB Stenungsund
: ECB - Existing Chemicals Ispra (VA)
: Hoechst AG Frankfurt/Main
: Celanese GmbH Frankfurt am Main
(63)

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 600 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : 29 mixed guinea pigs (strain not reported) received single doses of 2-ethylhexanol by gavage at levels of 0.5, 0.63, 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed

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Source : 0.795 and 1.26 g/kg. Gross necropsy evaluation revealed congestion of the spleen and liver as well as paleness of the kidney.

: Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(63)

5.1.2 ACUTE INHALATION TOXICITY

Type : other
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 4 hour(s)
Remark : Result: 2 groups of 6 Sprague-Dawley rats (3 male, 3 female) were exposed once to a vapor concentration of 0.89 mg/l and an aerosol/vapor concentration of 5.3 mg/l. Exposure was for 4 hrs, followed by a 7-day observation period. All animals exposed to 5.3 mg/l died within 48 hrs of exposure, while animals of the other exposure group survived.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(72)

Type : other
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: 99.5%
Remark : Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motility, slight to moderate dyspnoea, and moderate irritation of the eyes, nose, pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.

Source : Neste Oxo AB Stenungsund

(73)

Type : other
Species : rat
Strain :
Sex :

5. Toxicity

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Date 05.11.2001

Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: 99.5%
Remark : Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motility, slight to moderate dyspnoea, and moderate irritation of the eyes, nose, pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(59)

Type : other
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: 99.5%
Remark : Result: A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of toxicity were reduced motility, slight to moderate dyspnoea, and moderate irritation of the eyes, nose, pharynx and snout. The symptoms had subsided in rats 1 hour after exposure.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(59)

Type : other
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time :
Value : 44 ppm
Remark : Result: 44 ppm 2-ethylhexanol caused a 50% reduction in respiratory frequency in mice.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5. Toxicity

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Celanese GmbH Frankfurt am Main

(74)

Type : other
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source : Neste Oxo AB Stenungsund

(75)

Type : other
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(59)

Type : other
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

5. Toxicity

Id 104-76-7
Date 05.11.2001

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (59)

Type : other: Dampfinhalation
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time :
Method : other: interne Richtlinie der Hoechst AG
Year : 1951
GLP : no
Test substance : other TS
Remark : 2 ml Substanz in 7 Liter Luftraum verdampft rufen keine Letalität hervor.

Source : Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Test condition : Substanzreinheit > 98 % (76)

Type : other: Vapor inhalation
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time :
Method : other: guidelines of Hoechst AG
Year : 1951
GLP : no
Test substance : other TS
Remark : 2 ml of 2-Ethylhexanol (vapour) in 7 l of air resulted in no lethal effects.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Test condition : 2-Ethylhexanol concentration: > 98% (76)

Type : other
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour

5. Toxicity

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under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source : Neste Oxo AB Stenungsund (75)

Type : other
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (59)

Type : other
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 6 hour(s)
Method :
Year :
GLP : no
Test substance : other TS: purity 99.5%
Remark : A group of ten Swiss mice, Wistar rats and English Short Hair guinea pigs were exposed to 227 ppm 2-ethylhexanol under dynamic conditions for 6 hours, followed by a 24-hour holding period. No deaths were seen. Signs of systemic toxicity were not pronounced and consisted primarily of central nervous system depression.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (59)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :

5. Toxicity

Id 104-76-7
Date 05.11.2001

Value : > 3000 mg/kg bw
Method : OECD Guide-line 402 "Acute dermal Toxicity"
Year : 1981
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(77)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1980 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Source : Neste Oxo AB Stenungsund

(78)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 2600 mg/kg bw
Method :
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : 2-ethylhexanol did not produce any clinical signs of toxicity.
Source : Neste Oxo AB Stenungsund

(75)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1980 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(64)

Type : LD50

5. Toxicity

Id 104-76-7

Date 05.11.2001

Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 2600 mg/kg bw
Method :
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : 2-ethylhexanol did not produce any clinical signs of toxicity.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(59)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1980 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 2600 mg/kg bw
Method :
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : 2-ethylhexanol did not produce any clinical signs of toxicity.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(59)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :

5. Toxicity

Id 104-76-7
Date 05.11.2001

Vehicle :
Route of admin. : i.p.
Exposure time :
Value : = 937 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : Range of values: 860-1020 mg/kg.
2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund

(79)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : 568 - 739 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: 2-EH technical grade
Remark : Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 female rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(80)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : = 650 mg/kg bw
Method :
Year :
GLP : no
Test substance :
Remark : Rats promptly developed an irregular gait, dragging of hind legs, breathing became gasping, even on lower doses; rats were sound asleep in 10 min.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

5. Toxicity

Id 104-76-7
Date 05.11.2001

Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(81)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : = 937 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : Range of values: 860-1020 mg/kg.
2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(80)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : = 937 mg/kg bw
Method :
Year :
GLP :
Test substance : other TS: 2-EH technical grade
Remark : Range of values: 860-1020 mg/kg.
2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 male rats. The LD50 was calculated 1 day after the test substance administration (no further details reported).
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(80)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :

5. Toxicity

Id 104-76-7

Date 05.11.2001

Value : 845 - 939 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: 2-EH technical grade
Remark : Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 70 male mice. The LD50 was calculated 1 day after the administration of the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(80)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : 726 - 801 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: 2-EH technical grade
Remark : Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund

(82)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : 726 - 801 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: 2-EH technical grade
Remark : Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(80)

Type : LD50

5. Toxicity

Id 104-76-7
Date 05.11.2001

Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.p.
Exposure time :
Value : 726 - 801 mg/kg bw
Method :
Year :
GLP : no
Test substance : other TS: 2-EH technical grade
Remark : Method: 2-Ethylhexanol (technical grade) was diluted 1:5 in peanut oil and administered to a total of 50 femal mice. The LD50 was calculated 1 day after the test substance administration (no further details reported).

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(80)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : s.c.
Exposure time :
Method :
Year :
GLP : no
Test substance :
Remark : Range of values: 6.67-13.0 ml/kg (5.54-10.79 g/kg).
2-Ethylhexanol was given to female rats; no further details given.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification :
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1981
GLP : no

5. Toxicity

Id 104-76-7

Date 05.11.2001

Test substance : as prescribed by 1.1 - 1.4
Remark : Method :2-Ethylhexanol was applied under occlusion to the skin of 3 male rabbits for 4 hours.

Result: An irritation index of 6.75/8 was determined.
redness: x=3.33
edema : x=4.00

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification :
Method :
Year :
GLP : no
Test substance :
Remark : Method: Single dermal application, shaved dorsal skin, 24 hr occlusion.

Result: moderate irritation
(scale:slight-moderate-marked-severe)
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund

(75)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result :
EC classification :
Method :
Year :
GLP : no
Test substance :
Remark : Irritation Index: 3/10.
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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5. Toxicity

Id 104-76-7
Date 05.11.2001

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : highly irritating
EC classification :
Method : other: guidelines of Hoechst AG
Year : 1978
GLP : no
Test substance : no data
Remark : 0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.
Source : Neste Oxo AB Stenungsund

(84)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : BASF AG Ludwigshafen

(85)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : highly irritating
EC classification :
Method : other: interne Richtlinie der Hoechst AG
Year : 1978
GLP : no
Test substance : no data
Remark : 0.5 ml okklusiv auf die unverletzte Haut, Einwirkzeit 1, 2, 4 und 24 Stunden.
nicht einstuftbar, Reizerscheinungen nach 7 Tagen nicht reversibel.
Source : Hoechst AG Frankfurt/Main
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(86)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification :

5. Toxicity

Id 104-76-7
Date 05.11.2001

Method	:		
Year	:		
GLP	:	no	
Test substance	:		
Remark	:	Method: Single dermal application, shaved dorsal skin, 24 hr occlusion.	
		Result: moderate irritation (scale:slight-moderate-marked-severe) Not classifiable according to current EEC directives.	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(59)
Species	:	rabbit	
Concentration	:		
Exposure	:		
Exposure time	:		
Number of animals	:		
PDII	:		
Result	:	highly irritating	
EC classification	:		
Method	:	other: guidelines of Hoechst AG	
Year	:	1978	
GLP	:	no	
Test substance	:	no data	
Remark	:	0.5 ml of 2-Ethylhexanol was applied under occlusion on unabraded skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(86)
Species	:	rabbit	
Concentration	:		
Exposure	:		
Exposure time	:		
Number of animals	:		
PDII	:		
Result	:	moderately irritating	
EC classification	:		
Method	:		
Year	:		
GLP	:	no	
Test substance	:		
Remark	:	Method: Single dermal application, shaved dorsal skin, 24 hr occlusion.	
		Result: moderate irritation (scale:slight-moderate-marked-severe) Not classifiable according to current EEC directives.	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(59)
Species	:	rabbit	
Concentration	:		
Exposure	:		

5. Toxicity

Id 104-76-7
Date 05.11.2001

Exposure time :
Number of animals :
PDII :
Result : highly irritating
EC classification :
Method : other: guidelines of Hoechst AG
Year : 1978
GLP : no
Test substance : no data
Remark : 0.5 ml of 2-Ethylhexanol was applied under occlusion on unabrased skin for 1,2,4 and 24 hours. Irritation effects seen after 7 days were not reversible.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(86)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method : Draize Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days).
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund

(87)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : irritating
EC classification :
Method : OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year : 1981
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Irritation Index: 28.6/110
cornea: x=1.44
iris: x=0.89
conjunctiva: redness: x=2.56
chemosis: x=0.78

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

5. Toxicity

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Date 05.11.2001

Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(88)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method :
Year :
GLP : no
Test substance :
Remark : Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.
Source : Neste Oxo AB Stenungsund

(89)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method :
Year :
GLP : no data
Test substance : no data
Remark : The test substance was reported to be irritating to rabbit eyes; no details reported.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(90)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result :
EC classification :
Method : Draize Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days).

5. Toxicity

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	hrs), 0 (7 days). Not classifiable according to current EEC directives.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(59)
Species	: rabbit	
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	:	
Year	:	
GLP	: no	
Test substance	:	
Remark	: Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea. Not classifiable according to current EEC directives.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(64)
Species	: rabbit	
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	: Draize Test	
Year	:	
GLP	: no data	
Test substance	: as prescribed by 1.1 - 1.4	
Remark	: 2-Ethylhexanol resulted in the following median scores (based on the scoring system by Draize): 19 (24 hrs), 20 (72 hrs), 0 (7 days). Not classifiable according to current EEC directives.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(59)
Species	: rabbit	
Concentration	:	
Dose	:	
Exposure Time	:	
Comment	:	
Number of animals	:	
Result	:	
EC classification	:	
Method	:	
Year	:	
GLP	: no	
Test substance	:	
Remark	: Instillation into the conjunctival sac of 20 ug caused moderately severe irritation of the cornea.	

5. Toxicity

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moderately severe irritation of the cornea.
Not classifiable according to current EEC directives.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(64)

5.3 SENSITIZATION

Type : Patch-Test
Species : human
Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method : other: Maximization test
Year :
GLP : no
Test substance : no data
Remark : In an attempt to induce sensitization in 29 volunteers, subjects were given five 48-hr closed patch tests (during a 10-day period) with 4% in petrolatum. None of the subjects showed any positive reactions when challenged 10-14 days after the induction phase by final 48-hr closed patch test with the 4% petrolatum mixture.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(91)

5.4 REPEATED DOSE TOXICITY

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : inhalation
Exposure period : 90 days
Frequency of treatment : 6 hours/day, 5 days/week (total of 65 exposures)
Post obs. period : none
Doses : 0, 15, 40 and 120 ppm
Control group : yes
NOAEL : ≥ 120 ppm
Method : OECD Guide-line 413 "Subchronic Inhalation Toxicity: 90-day Study"
Year : 1981
GLP : yes
Test substance : other TS: purity 99.9%
Remark : 10 animals/sex/dose were used. The concentration of 120 ppm corresponds to the calculated saturated vapor concentration at 20°C. Body weights were determined weekly. Clinical signs and findings were recorded. Ophthalmologic examinations were carried out and blood was taken from all animals at the end of the 3-month exposure period. Numerous clinicochemical

5. Toxicity

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of the 3-month exposure period. Numerous clinicochemical and hematological parameters, and various enzyme activities were measured and a clotting time analysis was performed. The animals were sacrificed at the end of the 3-month exposure period and a complete necropsy of all animals including weighing of certain organs and a gross-pathologic evaluation was performed; selected organs/tissues were examined histologically.

Result : Under the conditions of the test no treatment-related toxic effects were found in male and female Wistar rats which were exposed to 2-ethylhexanol vapor up to 120 ppm.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : inhalation
Exposure period : 90 Tage
Frequency of treatment : 6 Std./Tag, 5 Tage/Woche
Post obs. period : keine
Doses : 0.081; 0.216; 0.648 mg/l (15; 40; 120 ppm) als Dampf
Control group : yes
NOAEL : .648 mg/l
Method : OECD Guide-line 413 "Subchronic Inhalation Toxicity: 90-day Study"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Je 10 maennliche und 10 weibliche Tiere wurden in die Kontroll- und Versuchsgruppen eingesetzt.
Es wurden in keiner Versuchsgruppe substanzbedingte Veraenderungen festgestellt. Untersucht wurden klinische, ophthalmologische, haematologische und klinisch-chemische Parameter. Nach Versuchsende wurden die Tiere pathologisch untersucht.

(92)

Source : BASF AG Ludwigshafen

(93)

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : inhalation
Exposure period : 14 Tage
Frequency of treatment : 6 Std./Tag, 5 Tage/Woche
Post obs. period : keine
Doses : 0.16; 0.32, 0.65 mg/l (30; 60; 120 ppm) als Dampf
Control group : yes
NOAEL : .32 mg/l
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Es handelte sich um eine Range-finding-study fuer einen 90-Tageversuch. Keine substanzbedingten Veraenderungen

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		90-Tageversuch. Keine substanzbedingten Veraenderungen wurden festgestellt, mit Ausnahme einer leichten Induktion der Cyanid-insensitiven Palmitoyl-CoA-Oxidase-Aktivitaet im Leberhomogenat der Tiere der hoechsten Dosisgruppe.	(94)
Source	:	BASF AG Ludwigshafen	
Species	:	rat	
Sex	:	male/female	
Strain	:	Fischer 344	
Route of admin.	:	oral feed	
Exposure period	:	11 days	
Frequency of treatment	:	daily	
Post obs. period	:	none	
Doses	:	0, 0.46%, 0.92%, 1.38%, 2.75% microencapsulated 2-ethylhexanol in the diet	
Control group	:	yes	
NOAEL	:	< .46 %	
LOAEL	:	= .46 %	
Method	:		
Year	:		
GLP	:	yes	
Test substance	:	other TS: purity 99.8%	
Remark	:	Control: placebo microcapsules (3%9 in the diet.	
Result	:	Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female rats per dose. The administration of 0.46, 0.92, 1.38 and 2.75 % (w/w) 2-ethylhexanol corresponded to a mean daily substance intake of about 500, 980, 1430, 2590 mg/kg bw 2-ethylhexanol in the male rat and of about 540, 1060, 1580, 2820 mg/kg body weight in the female rats. In all dose groups test substance related toxic effects were observed. Typical findings were: 0.46% group: increased relative stomach weights in the females; decreased cholesterol in both sexes; decreased triglycerides and alanine-aminotransferase in the males. 0.92% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute stomach weights in the females; decreased triglycerides and alanine-aminotransferase and increased total protein in the males; minimal diffuse hypertrophy of the hepatocytes in one female; slight diffuse hypertrophy of the hepatocytes in all male and female rats. 1.38% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute liver weights in both male and female animals; increase in the absolute stomach weights in the females; decreased cholesterol in both sexes; decreased triglycerides and alanine-aminotransferase in the males and decreased platelets in the females; increased total protein in the males; slight diffuse hypertrophy of the hepatocytes in most male and female rats; focal or multifocal acanthosis in the epithelium of the forestomach of one female rat. 2.75% group: increased relative liver and stomach weights in the animals of both sexes; increase in the absolute liver weights in the male and female animals; decreased cholesterol, triglycerides, glucose, alanine-aminotransferase, reticulocytes, platelets and mean	

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alanine-aminotransferase, reticulocytes, platelets and mean corpuscular volume in both sexes; focal or multifocal acanthosis in the epithelium of the forestomach in a few males and females.

Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(95)

Species : rat
Sex : male
Strain : Fischer 344
Route of admin. : oral feed
Exposure period : 3 weeks
Frequency of treatment : daily
Post obs. period : none
Doses : 2% in the diet
Control group : yes
Method :
Year :
GLP :
Test substance : no data
Result : Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACETYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.

Source : Neste Oxo AB Stenungsund

(96)

Species : rat
Sex : male/female
Strain : other: Dow-Wistar
Route of admin. : oral feed
Exposure period : 3 months
Frequency of treatment : daily
Post obs. period : none
Doses : 0.01, 0.05, 0.25, 1.25 % in the diet
Control group : yes
NOAEL : = .05 %
LOAEL : = .25 %
Method :
Year :
GLP : no
Test substance :
Result : Result: 10 male and 10 female rats per dose group were treated with 2-ethylhexanol. No mortality, appetite depression, body weight gain, or kidney weight effect was found associated with dosing. Typical findings were:

1.25% group: increased liver weights (absolute and relative) in both males and females; cortical degeneration of the kidney in the males; focal liver congestion and/or swelling in female rats; increased incidence and distribution of transitory hepatic diffuse cloudy swelling and also diffuse cloudy swelling of the proximal convoluted kidney tubules.

	cloudy swelling of the proximal convoluted kidney tubules.	
	0.25% group: A trend of the diffuse cloudy swelling of the liver and the kidney was suggested histologically although to a proportionally smaller degree, and believed to be fortuitous.	
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(97)
Species	: rat	
Sex	: male/female	
Strain	: Fischer 344	
Route of admin.	: oral feed	
Exposure period	: 11 Tage	
Frequency of treatment	: kontinuierlich	
Post obs. period	: keine	
Doses	: 1; 2; 3; 6 % in Mikrokapseln im Futter entspr. 0.46; 0.92; 1.38; 2.75 % 2-Ethylhexanol	
Control group	: yes, concurrent vehicle	
NOAEL	: < .46 %	
Method	: other	
Year	:	
GLP	: yes	
Test substance	: as prescribed by 1.1 - 1.4	
Result	: 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Kein Tier starb waehrend der Versuchsdauer. Die durchschnittliche taegliche Substanzaufnahme wurde fuer die weiblichen Tiere mit 500; 980; 1430 und 2590 mg/kg und fuer die maennlichen Tiere mit 540; 1060; 1580; 2820 mg/kg angegeben. In der 6 % Dosisgruppe wurde eine verminderte Trinkwasser- und Futteraufnahme waehrend der Versuchsdauer beschrieben. Das Koerpergewicht der Tiere war reduziert. Klinisch-chemische Untersuchungen erbrachten erniedrigte Werte von Cholesterol, Glucose und Alanin-Aminotransferase. Eine Abnahme von Reticulocyten, Thrombocyten und MCV wurde bei beiden Geschlechtern, von MCH bei weiblichen Tieren festgestellt. Ein Ansteigen des Gesamtproteingehaltes und der Erythrocyten wurde gemessen. Absolutes und relatives Lebergewicht waren erhoeht, wie auch das relative Magengewicht. Nur bei einem weiblichen Tier wurden makroskopisch fokale Laesionen im Vormagen festgestellt, mikroskopisch wurden bei mehreren Tieren Akanthose (fokal und multifokal) im Epithel des Vormagens beobachtet. Eine leichte diffuse Hypertrophie von Hepatocyten wurden bei allen Tieren dieser Dosisgruppe festgestellt. Auch in der 3 % und 2 % Dosisgruppe wurden die klinischen, klinisch-chemischen und haematologischen Veraenderungen, wie auch die pathologischen Organveraenderungen der hoechsten Dosisgruppe festgestellt. Auch in der 1 % Dosisgruppe wurde bei den maennlichen Tieren eine reduzierte Futteraufnahme beobachtet, auch waren die Veraenderungen bei den untersuchten klinisch-chemischen Parametern noch festzustellen. Bei den weiblichen Tieren war das relative Magengewicht erhoeht.	

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das relative Magengewicht erhoeht. Aufgrund der Befunde muss der NOAEL unterhalb der niedrigsten Dosierung liegen, d.h. < 0.46 % 2-Ethylhexanol.		
Source	: BASF AG Ludwigshafen	(98)
Species	: rat	
Sex	: male	
Strain	: Fischer 344	
Route of admin.	: oral feed	
Exposure period	: 3 weeks	
Frequency of treatment	: daily	
Post obs. period	: none	
Doses	: 2% in the diet	
Control group	: yes	
Method	:	
Year	:	
GLP	:	
Test substance	: no data	
Result	: Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(99)
Species	: rat	
Sex	: male	
Strain	: Fischer 344	
Route of admin.	: oral feed	
Exposure period	: 3 weeks	
Frequency of treatment	: daily	
Post obs. period	: none	
Doses	: 2% in the diet	
Control group	: yes	
Method	:	
Year	:	
GLP	:	
Test substance	: no data	
Result	: Result: Administration of 2-ethylhexanol (purity not reported) to rats induced a marked PROLIFERATION of HEPATIC PEROXISOMES together with a significant INCREASE in HEPATIC CATALASE and CARNITINE ACTEYLTRANSFERASE activity. SERUM TRIGLYCERIDES were significantly DECREASED.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(99)
Species	: rat	
Sex	: male/female	
Strain	: Fischer 344	
Route of admin.	: drinking water	
Exposure period	: 9 days	
Frequency of treatment	: daily	

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Post obs. period : none
Doses : 0, 308, 636 ppm
Control group : yes, concurrent vehicle
NOAEL : = 636 ppm
Method : other: according to TSCA and EPA guidelines
Year : 1983
GLP : yes
Test substance : other TS: purity >99.5%
Result : Result: Per dose, groups of 10 male and 10 female rats were exposed to 2-ethylhexanol. There were no treatment-related effects on clinical signs of toxicity, food consumption, body weight, serum chemistry, hematology, organ weights, gross pathology, or anatomic pathology.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(100)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 21 days
Frequency of treatment : daily
Post obs. period : none
Doses : 100, 300, 950 mg/kg/day (vehicle:corn oil)
Control group : yes, concurrent vehicle
LOAEL : 100 mg/kg
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Result : Result: Subchronic toxicity was evaluated in groups of 5 female and 5 male rats. There were no mortalities.

Clinical observations included reduced body weight gain in high dose females. Necropsy revealed elevated absolute and relative liver weights in high dose males and females in the 2 highest dose groups; elevated relative kidney weights in high dose females and males; increased serum triglyceride levels in high dose males; increased lauric acid 11 -and 12-hydroxylase activities in high dose females and males; a dose related reduction in neutral lipids in the livers of treated animals; a dose related increase in cyanide-insensitive palmitoyl CoA oxidation in females and males; slightly increased hepatic peroxisomes in high dose females and males.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

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Species	: rat
Sex	: male/female
Strain	: Fischer 344
Route of admin.	: gavage
Exposure period	: 3 months
Frequency of treatment	: daily (5 days /week)
Post obs. period	: none
Doses	: 25, 125, 250, 500 mg/kg (in aqueous emulsion)
Control group	: yes, concurrent vehicle
NOAEL	: = 125 mg/kg
LOAEL	: = 250 mg/kg
Method	:
Year	:
GLP	: yes
Test substance	: other TS: purity >99.8%
Remark	: Vehicle: bidistilled water containing 5 ug/ml Cremophor EL. Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed and samples of liver tissues and bone marrow were prepared for electron microscopy investigations; liver homogenates were prepared for clinicochemical examinations;
Result	: Result: Limited study: The oral administration of 2-ethylhexanol over a period of 3 months led to an impairment of feed consumption and body weight gain in the male and female animals of the 500 mg/kg dose group. The cyanide-insensitive palmitoyl CoA-oxidation in the liver of male and female rats was strongly induced in the 500 mg/kg dose group and less pronounced in the 250 mg/kg dose group, probably due to a proliferation of peroxisomes. No substance-related findings were observed in the other dose groups. NOEL: 125 mg/kg bodyweight LOEL: 250 mg/kg bodyweight Main study: Per dose group 10 male and 10 female rats were treated. After the 3-month administration of 2-ethylhexanol toxic effects occurred in male and female rats of the 500 and 250 mg/kg dose groups. Typical findings were: 25 and 125 mg/kg groups: no substance-related findings 250 mg/kg group: increased relative liver weights in both sexes; increased relative stomach weights in females; decrease in alkaline phosphatase and glucose in males; decrease in alanine-aminotransferase in female rats. 500 mg/kg group: increased relative liver and stomach weights in both sexes; increased relative liver weights in the animals of both sexes; increased absolute stomach weights in female rats; decrease in alanine-aminotransferase, glucose and cholesterol in both sexes; decrease in alkaline phosphatase in males; single or multiple slightly elevated foci in the mucosa of the forestomach of male and female rats; focal or multifocal acantosis in the mucosa of the forestomach of one male and

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	acantosis in the mucosa of the forestomach of one male and five female animals.	
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(102)
Species	: rat	
Sex	: male	
Strain	: Wistar	
Route of admin.	: gavage	
Exposure period	: 7 days	
Frequency of treatment	: daily	
Post obs. period	: none	
Doses	: 0, 1335 mg/kg/day in corn oil	
Control group	: yes, concurrent vehicle	
Method	:	
Year	:	
GLP	: no	
Test substance	: no data	
Result	: Result: The oral administration of 1335 mg/kg 2-ethylhexanol to a group of 6 male Wistar rats resulted in increased relative liver weights as compared to the control. In addition, significantly increased activity of cytochrome P-450s and biphenyl-4-hydroxylase of the liver were observed. Microsomal glucose-6-phosphatase activity was significantly decreased, while liver succinate dehydrogenase and aniline-4-hydroxylase activities were similar to the control. In the liver, electronmicroscopy studies showed and increase in the number of peroxisomes and dilatation of the smooth endoplasmic reticulum.	
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(103)
Species	: rat	
Sex	: male	
Strain	: Sprague-Dawley	
Route of admin.	: gavage	
Exposure period	: 5 days	
Frequency of treatment	: daily	
Post obs. period	:	
Doses	: 352 mg/kg	
Control group	:	
Result	: Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.	

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Source	: Neste Oxo AB Stenungsund	(104)
Species	: rat	
Sex	: male/female	
Strain	: Fischer 344	
Route of admin.	: gavage	
Exposure period	: 11 days (9 applications)	
Frequency of treatment	: 5 days/week	
Post obs. period	: none	
Doses	: 0, 100, 330, 1000, 1500 mg/kg (in aqueous emulsion)	
Control group	: yes, concurrent vehicle	
NOAEL	: = 100 mg/kg	
LOAEL	: 330 mg/kg	
Method	:	
Year	:	
GLP	: yes	
Test substance	: other TS: purity >99.8%	
Remark	: vehicle: bidistilled water containing 5 ul/100 ml Cremophor EL.	
Result	<p>: Result: Per dose 10 male and 10 female animals were treated. The 9-fold administration of 2-ethylhexanol to rats at doses of 1000 and 1500 mg/kg body weight led to clear toxic signs like impairment of food consumption and body weight gain as well as ataxia and/or lethargy. No substance-related effects were observed in the 100 mg/kg dose group.</p> <p>1500 mg/kg dose group: decrease of cholesterol, glucose and reticulocytes in the animal of both sexes; increase of alanine aminotransferase in the males; increased relative stomach, liver, kidney and brain weights and decreased relative spleen weights in both sexes; increased relative adrenal weight in the male and lung weight in the female animals; foci in the forestomach of 4 male and 7 female animals; hyperkeratosis and focal or multifocal acanthosis in the mucous membrane of the forestomach of all rats as well as epithelial degeneration, ulceration and subcutaneous inflammatory edema in some animals; slight hypertrophy of hepatocytes in the liver of 8 male and female rats each; focal hepatocellular necrosis in 2 male and 1 female rat; parenchymal involution of lympho-reticular tissue in the spleen in both sexes; decreased thymus size and lymphocyte depletion and necrosis in animals of both sexes.</p> <p>1000 mg/kg dose group: decrease of cholesterol and reticulocytes in both sexes; increased relative stomach, liver and kidney weights and decreased spleen weights in both sexes; increased relative brain weight in the female rats; foci in the forestomach of 2 males; hyperkeratosis and focal or multifocal acanthosis in the mucous membrane of the forestomach of most male and female rats as well as epithelial degeneration, ulceration and subcutaneous inflammatory edema; parenchymal involution of lymphoreticular tissue in the spleen of 5 female rats; decreased thymus size in 2 male and 5 female rats; lymphocyte depletion and necrosis in the thymus of some female rats.</p> <p>330 mg/kg dose group: increased relative kidney weights of the female rats; inflammatory edema in the forestomach of 1 female and</p>	

Source	<p>inflammatory edema in the forestomach of 1 female and decreased thymus size in 2 male and 1 female rat.</p> <p>: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(105)
Species	: rat	
Sex	: male/female	
Strain	: Fischer 344	
Route of admin.	: gavage	
Exposure period	: 9 days	
Frequency of treatment	: 5 days + 2 days without treatment + 4 days	
Post obs. period	: none	
Doses	: 0.1, 0.33, 1.0, 1.5 ml/kg/day (=83, 275, 834, 1250 mg/kg/day)	
Control group	: yes	
NOAEL	: 83 mg/kg	
Method	: other: according to TSCA and EPA guidelines	
Year	: 1983	
GLP	: yes	
Test substance	: other TS: purity >99.5%	
Result	<p>: Result: Per dose, groups of 10 male and 10 female F-344 rats were exposed by oral gavage to 2-ethylhexanol (undiluted). Treatment resulted in a spectrum of treatment-related, dose-dependent toxic effects in male and female rats.</p> <p>No treatment-related effects were observed for any in-life, clinical pathology, gross necropsy, or histopathology observations at the 0.1 ml/kg/day level.</p> <p>Effects associated with the administration of 2-ethylhexanol in males and/or females at one or more of the three highest dose levels were decreased food consumption and body weights, decreased total leukocytes and lymphocytes, increased liver weight, increased stomach weight (associated with hyperkeratosis, mucosal hyperplasia, edema, exocytosis and gastritis of the forestomach, but not glandular stomach), decreased spleen weight, thymic atrophy and lymphoid cell degeneratiion.</p>	
Source	<p>: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(100)
Species	: rat	
Sex	: male/female	
Strain	: Fischer 344	
Route of admin.	: gavage	
Exposure period	: 11 days (9 applications)	
Frequency of treatment	: 5 days/week	

5. Toxicity

Id 104-76-7

Date 05.11.2001

Post obs. period	:	none
Doses	:	0, 100, 330, 1000, 1500 mg/kg (in propylene glycol)
Control group	:	yes, concurrent vehicle
NOAEL	:	< 100 mg/kg
LOAEL	:	= 100 mg/kg
Method	:	
Year	:	
GLP	:	yes
Test substance	:	other TS: purity >99.8%
Remark	:	Vehicle: propylene glycol
Result	:	<p>Per dose group, 10 male and 10 female rats were treated. 1500 mg/kg b.w. 2-ethylhexanol proved to be lethal for all female animals and 6 of the male animals. Doses of 1500, 1000, and 330 mg/kg bw resulted in clinically observable toxic effects like lethargy, ataxia, and/or reduced food consumption accompanied by reduced body weight gain.</p> <p>1500 mg/kg group: Extremely reduced feed consumption and body weight in the surviving males; decrease of cholesterol, alanine-aminotransferase, leucocytes, lymphocytes, monocytes, hemoglobin, hematocrit, meancell volume, mean corpuscular hemoglobin and reticulocytes; increase in neutrophilic polymorpho-nuclear granulocytes; increase in relative stomach, liver and kidney weights and decrease in relative spleen and testes weights; foci in the forestomach.</p> <p>1000 mg/kg dose group: Reduced feed consumption and body weight in the animals of both sexes; decrease of cholesterol, alanine-aminotransferase, leucocytes, lymphocytes, monocytes, hemoglobin, hematocrit, mean cell volume and reticulocytes and increase of the neutrophilic polymorphonuclear granulocytes in both sexes; decrease of the mean corpuscular hemoglobin in the males; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased testes weights in males; foci in the forestomach of all animals and ulcer in the forestomach of 2 males.</p> <p>330 mg/kg group: Decrease of alanine-aminotransferase, hemoglobin, hematocrit, mean cell volume and reticulocytes and increase in the neutrophilic polymorphonuclear granulocytes in the females; increased relative stomach weight in both sexes, increased relative liver weight in the female and increased testes weights in the male animals; foci in the forestomach of all animals.</p> <p>100 mg/kg group: Decreased of alanine-aminotransferase in the females; decreased relative liver weights in the male animals.</p>
Source	:	<p>Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>

(106)

5. Toxicity

Id 104-76-7

Date 05.11.2001

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 11 days (9 applications)
Frequency of treatment : 5 days /week
Post obs. period : none
Doses : 100, 330, 1000, 1500 mg/kg (in corn oil)
Control group : yes, concurrent vehicle
NOAEL : = 100 mg/kg
LOAEL : = 330 mg/kg
Method :
Year :
GLP : yes
Test substance : other TS: purity >99.8%
Result : Per dose 10 male and 10 female animals were treated. The 9-fold administration of 2-ethylhexanol to rats at doses of 1000 and 1500 mg/kg bw led to clear toxic signs like impairment of food consumption and body weight gain as well as ataxia and/or lethargy, piloerection, and genital region smeared with urine in both sexes. Some of these toxic signs were also found in some animals of the 330 mg/kg dose group.

1500 mg/kg dose group:

One female rat died during the conduct of the study; decrease of cholesterol, glucose, alanine-aminotransferase, leukocytes, lymphocytes, monocytes and reticulocytes in both sexes; lowering of mean cell volume and mean corpuscular hemoglobin in the females; increase in total protein and triglycerides in both sexes; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased relative testes weights; thickening of the wall of the forestomach and foci in the forestomach in some males and females.

1000 mg/kg dose group:

One male rat died during the conduct of the study; decrease of cholesterol, glucose, leukocytes, lymphocytes and reticulocytes in both sexes; decrease of monocytes and increase of total protein in the males and decrease of the mean cell volume in the females; increased relative stomach, liver and kidney and decreased relative spleen weights in both sexes; increased relative testes weights; thickening of the wall and foci in the forestomach in some animals.

330 mg/kg dose group:

Increased relative testes weights; thickening of the wall and foci in the forestomach in some animals.

100 mg/kg dose group:

No substance-related findings.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(107)

5. Toxicity

Id 104-76-7

Date 05.11.2001

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 11 Tage
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post obs. period : keine
Doses : 100; 330; 1000; 1500 mg/kg in Maisoel appliziert
Control group : yes, concurrent vehicle
NOAEL : 100 - 330 mg/kg
LOAEL : 330 mg/kg
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Testsubstanz wurde in 5 ml/kg Maisoel appliziert. In der 1500 mg/kg Dosisgruppe starb ein weibliches Tier waehrend der Versuchsdauer, in der 1000 mg/kg Dosisgruppe ein maennliches Tier.
In der hoechsten Dosisgruppe waren Futteraufnahme und Koerpergewichtsentwicklung reduziert. Ataxie, gestraeubtes Fell und bei einigen Tieren Lethargie und Speichelfluss wurden beobachtet. Bei 9 weiblichen Tieren und einem maennlichen Tier war in der Genitalregion das Fell mit Urin verklebt. Klinisch-chemische und haematologische Untersuchungen zeigten reduzierte Cholesterin-, Glucose- und Alanin-Aminotransferase-Werte. Gesamtproteingehalt und Triglyceride waren erhoeht. Leukocyten-, Lymphocyten-, Monocyten und Reticulocytenzahl war verringert, bei den weiblichen Tieren war auch das mittlere Blutkoerperchenvolumen und der Hb-Faerbkoeffizient verringert. Die absoluten Organgewichte von Leber und Milz waren bei beiden Geschlechtern reduziert, die von Niere und Hoden waren bei den maennlichen Tieren reduziert, vom Magen erhoeht. Relativ waren Magen-, Leber- und Nierengewicht bei beiden Geschlechtern erhoeht und Milzgewicht verringert. Das relative Hodengewicht war erhoeht. Histologisch wurde eine Verdickung der Vormagenwand, bei einigen Tieren mit Focibildung, beschrieben.
In der 1000 mg/kg Dosisgruppe wurden im wesentlichen noch die gleichen Symptome wie in der 1500 mg/kg Dosisgruppe beobachtet.
330 mg/kg bewirkten Ataxie, gestraeubtes Fell und Urin auf dem Fell im Genitalbereich nur noch bei einigen Tieren. Es wurden keine klinisch-chemischen wie auch haematologischen Veraenderungen festgestellt. Das relative Hodengewicht war erhoeht. Die Veraenderungen im Vormagen wurden nur noch bei 3 Tieren festgestellt.
Bei den Tieren, die 100 mg/kg erhielten wurden keine substanzbedingten Veraenderungen festgestellt.

Source : BASF AG Ludwigshafen

(108)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 11 Tage

5. Toxicity

Id 104-76-7

Date 05.11.2001

Frequency of treatment	: einmal taeglich, 5 Tage/Woche
Post obs. period	: keine
Doses	: 100; 330; 1000; 1500 mg/kg in Propylenglykol appliziert
Control group	: yes, concurrent vehicle
NOAEL	: < 100 mg/kg
Method	: other
Year	:
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Result	: <p>Je 10 maennliche und 10 weibliche Tiere wurden in die Versuchs- und Kontrollgruppen eingesetzt. Die Substanz wurde in je 5 ml/kg Propylenglykol appliziert.</p> <p>In der 1500 mg/kg Dosisgruppe starben alle weiblichen und 6 maennliche Tiere. Die Futteraufnahme und die Koerpergewichtsentwicklung der ueberlebenden Tiere war signifikant reduziert, die Trinkwasseraufnahme erhoeht. Ataxie, Lethargie, gestraeubtes Fell, Bewusstseinsverlust, Hypothermie und bei einigen Tieren Speichelfluss und Urin auf dem Fell im Genitalbereich wurden als klinische Veraenderungen beschrieben. Bei den ueberlebenden Tieren waren im Blut Cholesterin, die Alanin-Aminotransferase, Leukocyten, Lymphocyten, Monocyten, Haemoglobin, Haematokrit, MCV und MCH reduziert, neutrophile polymorphkernige Granulocyten erhoeht. Die relativen Magen-, Leber- und Nierengewichte waren erhoeht, relative Hoden- und Milzgewichte verringert. Absolut waren Magen- und Lebergewichte erhoeht, Milz- und Nierengewichte reduziert. Bei allen ueberlebenden Tieren wurden Foci im Vormagen festgestellt.</p> <p>2 Tiere der 1000 mg/kg Dosisgruppe starben. Klinische, klinisch-chemische und haematologische Veraenderungen entsprachen im wesentlichen denen, die bei den ueberlebenden Tieren der 1500 mg/kg Dosisgruppe beschrieben wurden.</p> <p>In der 330 mg/kg Dosisgruppe wurden bei je 3 maennlichen und 3 weiblichen Tieren noch klinische Veraenderungen in Form von Ataxie und Lethargie beschrieben. Auch waren die klinisch-chemischen und haematologischen Parameter noch veraendert. Absolute und relative Magen- und Hodengewichte waren erhoeht, wie auch die relativen Lebergewichte bei weiblichen Tieren. Bei allen Tieren wurde Focibildung im Vormagen beschrieben.</p> <p>In der 100 mg/kg Dosisgruppe waren bei den weiblichen Tieren die Alanin-Aminotransferase vermindert. Bei den maennlichen Tieren wurden verringerte relative Lebergewichte beschrieben. Keine weiteren substanzbedingten Veraenderungen wurden festgestellt.</p> <p>Der NOEAL liegt unter 100 mg/kg.</p>
Source	: BASF AG Ludwigshafen

(109)

Species	: rat
Sex	: male/female
Strain	: Fischer 344
Route of admin.	: gavage
Exposure period	: 11 Tage
Frequency of treatment	: einmal taeglich, 5 Tage/Woche
Post obs. period	: keine
Doses	: 100; 330; 1000; 1500 mg/kg in waessriger Emulsion appliziert
Control group	: yes, concurrent vehicle

NOAEL	: 100 - 330 mg/kg
Method	: other
Year	:
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Result	: Je 10 maennliche und 10 weibliche Tiere wurden in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert dem 5 ul/100 ml Cremophor EL zugesetzt waren. Kein Tier starb waehrend der Versuchsdauer. In der 1500 mg/kg Dosisgruppe war die Futteraufnahme und das Koerpergewicht der Tiere reduziert. Klinische Veraenderungen waren Ataxie, Lethargie, z.T. erschienen die Tiere bewusstlos, gestraeubtes Fell und Urin auf dem Fell im Genitalbereich. Die Cholesterol- und Glucosewerte waren reduziert, die Alanin-Aminotransferase bei den maennlichen Tieren erhoeht. Die Reticulocytenzahl war vermindert. Das absolute Organgewicht von Milz, Gehirn und Nebenniere war reduziert, das von Leber und Magen erhoeht. Relativ waren Magen-, Nieren-, Leber- und Gehirngewicht erhoeht, das relative Nebennierengewicht war bei den maennlichen Tieren und das relative Lungengewicht bei den weiblichen Tieren erhoeht. Das relative Milzgewicht war bei beiden Geschlechtern reduziert. Makroskopisch wurden im Vormagen bei den meisten Tieren Foci festgestellt. Histologisch wurden Hyperkeratosen, Akanthosen (fokal, multifokal) in der Vormagenschleimhaut bei allen Tieren beschrieben, bei einigen Tieren wurden epitheliale Degenerationen, Ulcerationen und subkutane entzuendliche Oedeme beschrieben. Bei einigen Tieren wurde eine leicht Hypertrophie der Hepatocyten, fokale hepatocellulaere Nekrosen und eine Rueckbildung des lymphoreticularen Gewebes festgestellt. Eine Verminderung der Thymusgroesse wurde bei fast allen Tieren beobachtet, wie auch eine Lymphocytendepletion im Thymus, bei einigen Tieren Lymphocytennekrosen. In der 1000 mg/kg Dosisgruppe wurden die gleichen Veraenderungen wie in der hoechsten Dosisgruppe beschrieben. In der 330 mg/kg Dosisgruppe waren die relativen Nierengewichte der weiblichen Tiere erhoeht. Die Thymusgroesse war bei 3 Tieren vermindert, bei einem weiblichen Tier wurden entzuendliche Oedeme im Vormagen festgestellt. Keine weiteren substanzbedingten Veraenderungen wurden beschrieben. 100 mg/kg bewirkte keine substanzbedingten Effekte.
Source	: BASF AG Ludwigshafen

(110)

Species	: rat
Sex	: male/female
Strain	: Fischer 344
Route of admin.	: gavage
Exposure period	: 3 Monate
Frequency of treatment	: einmal taeglich, 5 Tage/Woche
Post obs. period	: keine
Doses	: 25; 125; 250; 500 mg/kg als waessrige Emulsion appliziert
Control group	: yes, concurrent vehicle
NOAEL	: 125 - 250 mg/kg
Method	: other
Year	:
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4

Result	<p>: Je 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg Wasser appliziert, dem 5 ul/100 ml Cremophor EL zugesetzt waren. Keine Tiere starben waehrend der Versuchsdauer.</p> <p>In der hoechsten Dosisgruppe war sowohl die Koerpergewichtsentwicklung wie auch das Koerpergewicht der Tiere reduziert. Alanin-Aminotransferase, Glucose- und Cholesterolspiegel waren vermindert bei beiden Geschlechtern, bei den maennlichen Tieren war die alkalische Phosphatase vermindert, der Gesamtprotein- und Albumingehalt erhoeht. Ein Ansteigen der Reticulocyten wurde beschrieben. Absolute und relative Magen- und Lebergewichte waren erhoeht. Focibildung in der Schleimhaut des Vormagens wurde beschrieben. Histologisch wurden bei einigen Tieren Akanthose der Mucosa im Vormagen beschrieben. Bei einigen Tieren traten fettige Infiltrationen in der Leber (lobulaere Peripherie) auf.</p> <p>In der 250 mg/kg Dosisgruppe wurden keine klinischen Veraenderungen festgestellt. Bei den maennlichen Tieren waren die alkalische Phosphatase und der Glucosespiegel reduziert, bei weiblichen Tieren die Alanin-Aminotransferase erhoeht. Das relative Lebergewicht war bei beiden Geschlechtern erhoeht, das relative Magengewicht nur bei weiblichen Tieren. Bei mikroskopischen Untersuchungen wurden geringgradige Fetteinlagerungen in den Leberzellen festgestellt.</p> <p>In der 125 und 25 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.</p> <p>Es wurde zusaetzlich eine Satellitenstudie mit je 3 maennlichen und weiblichen Tieren pro Versuchs- und Kontrollgruppe durchgefuehrt. Bei diesen Tieren wurde nach Versuchsende das Leber- und Knochenmarkgewebe fuer elektronenmikroskopischen Untersuchungen praepariert. Sowohl in der 250 wie auch 500 mg/kg wurde bei beiden Geschlechtern dosisabhaengig eine Induktion der Cyanid-resistenten (peroxisomalen) Palmitoyl -CoA-Oxidase festgestellt.</p>	
Source	: BASF AG Ludwigshafen	(111) (112)
Species	: rat	
Sex	: male	
Strain	: Sprague-Dawley	
Route of admin.	: gavage	
Exposure period	: 5 days	
Frequency of treatment	: daily	
Post obs. period	:	
Doses	: 352 mg/kg	
Control group	:	
Result	<p>: Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(113)
Species	: rat	

5. Toxicity

Id 104-76-7
Date 05.11.2001

Sex : male
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 5 days
Frequency of treatment : daily
Post obs. period :
Doses : 352 mg/kg
Control group :
Result : Result: In this study an examination was made of the effect of 2-ethylhexanol on body weight, liver weights and on testicular and prostate weight. The seminiferous tubules were examined histologically. No indications were found of any changes.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(113)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : dermal
Exposure period : 9 days
Frequency of treatment : 5 days treatment, 2 days no treatment, 4 days treatment
Post obs. period : none
Doses : 0, 0.5, 1.0 ml/kg/day (=0, 417, 834 mg/kg/day)
Control group : yes
Method : other: according to TSCA and EPA guidelines
Year : 1983
GLP : yes
Test substance : other TS: purity >99.5%
Remark : Control: water
Result : Result: Per dose, groups of 10 male and 10 female F-344 rats were exposed to 2-ethylhexanol (undiluted, occluded cutaneous). Exposure was for 6 hours per treatment day. There were no treatment-related effects on clinical signs of toxicity, food consumption, or body weight following cutaneous exposure to 2-ethylhexanol. Lymphopenia and decreased spleen weight for high dose females and increased triglycerides for females at both dose levels compared to controls were observed. No other treatment-related effects on clinical pathology measurements or organ weights were observed for males or females at either dose level. Treatment-related anatomic and histologic lesions observed following cutaneous exposure to 2-ethylhexanol were restricted to the site of application and included exfoliation, acanthosis, hyperkeratosis, eschar formation, dermatitis and edema.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(100)

Species : rat

5. Toxicity

Id 104-76-7

Date 05.11.2001

Sex : male
Strain : other
Route of admin. : dermal
Exposure period : 16 days
Frequency of treatment : 5 days/week
Post obs. period : 14 days
Doses : 0, 2.0 ml/kg/day
Control group : yes, concurrent no treatment
Method :
Year :
GLP : no
Test substance :
Result : Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period).

On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced.

There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum.

Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls):

Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration.

Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis.

Kidneys: Epithelial-cell necrosis, cysts, basophilic "balloon nuclei".

Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema.

Testes: interstitial oedema, reduced spermiogenesis.

Thymus: increased "colliodocytes".

Adrenals: Cortex very rich in lipoids.

Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.

Source : Neste Oxo AB Stenungsund

(114)

Species : rat
Sex : male
Strain : other
Route of admin. : dermal
Exposure period : 16 days
Frequency of treatment : 5 days/week
Post obs. period : 14 days
Doses : 0, 2.0 ml/kg/day

5. Toxicity

Id 104-76-7

Date 05.11.2001

Control group	: yes, concurrent no treatment
Method	:
Year	:
GLP	: no
Test substance	:
Result	: Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period). On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced. There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum. Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls): Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration. Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis. Kidneys: Epithelial-cell necrosis, cysts, basophilic "ballon nuclei". Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema. Testes: interstitial oedema, reduced spermiogenesis. Thymus: increased "colliodocytes". Adrenals: Cortex very rich in lipoids. Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main
Species	: rat
Sex	: male
Strain	: other
Route of admin.	: dermal
Exposure period	: 16 days
Frequency of treatment	: 5 days/week
Post obs. period	: 14 days
Doses	: 0, 2.0 ml/kg/day
Control group	: yes, concurrent no treatment
Method	:
Year	:
GLP	: no
Test substance	:
Result	: Result: 2.0 ml/kg/day 2-ethylhexanol (undiluted technical grade) was applied to the shaved back skin fo rats.

(80)

grade) was applied to the shaved back skin fo rats. Application was non occlusive, the animals were immobilized for two hours after the application. 5 animals were killed on the 17th day (the end of treatment period) and the remaining 5 on the 30th day (the end of observation period).

On the 10th day a slight reddening and crusting of the skin was evident. The body weights on the 9th and 10th day, and the relative and absolute thymus weights on the 17th day, were significantly reduced.

There were no effects on the weights of the heart, liver, spleen, or kidney, the level of protein, albumin, alpha-1-,beta-1-, and gamma-globulin content in serum.

Histologically the following effects on organs were observed (with at least 3 out of 5 treated animals differing from the controls):

Liver: histiocytic and inflammatory granulomas, peripheral fine-droplet fatty degeneration.

Lungs: interstitial pneumonia, bronchiectasis, severe round-cell bronchitis.

Kidneys: Epithelial-cell necrosis, cysts, basophilic "balloon nuclei".

Heart: inter- and intracellular oedema, necrobiotic muscle fibres, interstitial oedema.

Testes: interstitial oedema, reduced spermiogenesis.

Thymus: increased "colliodocytes".

Adrenals: Cortex very rich in lipoids.

Histochemical investigation of the liver showed raised succinate-dehydrogenase activity and reduced lactate dehydrogenase activity. Tests on acid phosphatase and non-specific alpha-naphtylacetate esterase activity and on fat coloration gave no indications of any changes.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(80)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : oral feed
Exposure period : 11 days
Frequency of treatment : daily
Post obs. period : none
Doses : 0.22, 0.44, 0.66, 1.32 % microencapsulated in the diet
Control group : yes, concurrent vehicle
NOAEL : = .44 - .66 %
LOAEL : = .66 - 1.32 %
Method :
Year :
GLP : yes
Test substance : other TS: purity >99.8%
Remark : NOEL: 0.44% = 1150 mg/kg/d (males)
0.66% = 2650 mg/kg/d (females)

Control: placebo microcapsules (1.5%) in the diet.

5. Toxicity

Id 104-76-7

Date 05.11.2001

Result : Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. The administration of 0.22, 0.44, 0.66 and 1.32 % 2-ethylhexanol in the diet corresponded to a mean daily intake of about 550, 1150, 1800 and 4450 mg/kg b w 2-ethylhexanol for male mice and of about 750, 1750, 2650 and 5750 mg/kg bw for female mice. The only effect that could be assessed to be a substance related finding was the reduction in body weight gain in the male animals of the 0.66% group.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(115)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : oral feed
Exposure period : 11 Tage
Frequency of treatment : kontinuierlich
Post obs. period : keine
Doses : 0.48; 0.96; 1.44; 2.88 % in Mikrokapseln im Futter, entspr. 0.22; 0.44; 0.66; 1.32 % 2-Ethylhexanol
Control group : yes, concurrent vehicle
NOAEL : .44 - .66 %
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Es wurden je 10 maennliche und 10 weibliche Tiere in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanzaufnahme wurde fuer die weiblichen Tiere mit 750; 1750; 2650 und 5750 mg/kg angegeben, fuer die maennlichen Tiere mit 550; 1150; 1800 und 4450 mg/kg. Kein Tier starb waehrend der Versuchsdauer. In der hoechsten Dosisgruppe wurde bei beiden Geschlechtern eine verminderte Koerpergewichtsentwicklung festgestellt, in der zweithoechsten Dosierung wurde dieses nur noch bei den maennlichen Tieren beobachtet. Es traten keine weiteren substanzbedingten Veraenderungen auf, untersucht wurden sowohl klinisch-chemisch und haematologisch Parameter, wie auch moegliche Organveraenderungen. Der NOEL wurde von den Autoren zwischen 0.44 und 0.66 % fuer maennliche Tiere und zwischen 0.66 und 1.32 % fuer weibliche Tiere angegeben. Der NOAEL liegt bei 1.32 % 2-Ethylhexanol.

Source : BASF AG Ludwigshafen

(116)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 days (9 applications)
Frequency of treatment : daily (9 applications)
Post obs. period : none

5. Toxicity

Id 104-76-7

Date 05.11.2001

Doses : 0, 100, 330, 1000, 1500 mg/kg (in corn oil)
Control group : yes, concurrent vehicle
NOAEL : = 330 - 1000 mg/kg bw
LOAEL : = 1000 - 1500 mg/kg bw
Method :
Year :
GLP : yes
Test substance : other TS: purity >99.8%
Remark : NOEL: 330 mg/kg (males)
1000 mg/kg (females)
Result : Result: 2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose.
In the 1500 mg/kg dose group 1 male mouse died, 10 male and 5 female mice had clinical signs as ataxia, piloerection and lethargy. A few animals showed abdominal position and loss of consciousness. An increase in the absolute and relative stomach weights was observed in male and female mice. In addition, male mice had decreased absolute and relative testes weights, and the relative liver and kidney weights of female mice were decreased. Gross lesions (foci in the mucosa) were seen in the forestomach of 7 male and 2 female mice.

In the 1000 mg/kg dose group, a decrease in absolute and relative testes weights was observed.

In the 100 and 330 mg/kg groups no substance-related findings were observed.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(117)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 3 months
Frequency of treatment : 5 days per week
Post obs. period : none
Doses : 25, 125, 250, 500 mg/kg (aqueous emulsion)
Control group : yes, concurrent vehicle
NOAEL : = 125 - 250 mg/kg
LOAEL : 250 - 500 mg/kg
Method :
Year :
GLP : yes
Test substance :
Remark : Vehicle: bidistilled water containing 5 ug/100 ml Cremophore EL.
Concurrently to the main study a limited study with the same dosing regimen using 3 animals/sex/dose was performed; at the end of the treatment period all animals were sacrificed for electron microscopic investigations; liver homogenates were prepared for clinicochemical examinations.
Result : Results:

Limited study: At the end of the 3-month administration period there were no substance-related clinical findings. There was no increase in the activity of the cyanide-insensitive palmitoyl-CoA-oxidation in the liver of the animals in all dose groups.

Main study: NOEL (females) = 250 mg/kg
NOEL (males) = 125 mg/kg

2-Ethylhexanol was administered to groups of 10 male and 10 female mice per dose. After the 3-month administration of 2-ethylhexanol toxic effects affecting the stomach (increased weight and slight focal and multifocal acanthosis in the mucosa of the forestomach) occurred in the male and female animals of the 500 mg/kg dose group and in the male animals (increased relative weight) of the 250 mg/kg dose group. Clinically, none of the animals showed any abnormal signs which could be related to the test substance administration. No substance-related effects occurred regarding the clinical chemistry or hematology.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(118)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 days (9 applications)
Frequency of treatment : 5 days/week
Post obs. period : none
Doses : 0, 100, 330, 1000, 1500 mg/kg in propylene glycol
Control group : yes, concurrent vehicle
NOAEL : = 100 mg/kg
LOAEL : = 330 mg/kg
Method :
Year :
GLP : yes
Test substance : other TS: purity >99.8%
Result : Per dose group, 10 male and 10 female animals were treated. 1500 mg/kg and 1000 mg/kg 2-ethylhexanol being administered for 11 days (9 applications) proved to be a lethal dose for 4 male and 6 female (1500 mg/kg) or for 1 male and 1 female animal (1000 mg/kg), respectively. Doses of 1500 and 1000 mg/kg body weight resulted in clinically observable toxic effects like lethargy, ataxia, and/or reduced food consumption. Clinical chemistry and hematology did not show changes that could be related to the test substance administration.

1500 mg/kg dose group:
Increase relative stomach and liver weights in both sexes; increased relative spleen weight in female and decreased testes weights in the male mice; gross lesions (foci of the mucosa, mainly white colored and slightly

	(foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of the surviving animals of both sexes.
	1000 mg/kg dose group: Increased relative stomach and liver weights in both sexes; increased relative spleen weights in males; gross lesion (foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of the surviving animals of both sexes.
	330 mg/kg dose group: Increased relative stomach and liver weights in the males; gross lesions (foci of the mucosa, mainly white colored and slightly prominent) in the forestomach of both sexes.
	100 mg/kg dose group: No substance-related findings
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
	(119)
Species	: mouse
Sex	: male/female
Strain	: B6C3F1
Route of admin.	: gavage
Exposure period	: 11 days (9 applications)
Frequency of treatment	: 5 days/week
Post obs. period	: none
Doses	: 0, 100, 330, 1000, 1500 mg/kg (aqueous emulsion)
Control group	: yes, concurrent vehicle
NOAEL	: = 100 mg/kg
LOAEL	: = 330 mg/kg
Method	:
Year	:
GLP	: yes
Test substance	: other TS: >99.8%
Remark	: Vehicle: bidistilled water containing 5 ug/100ml Cremophor EL
Result	: Per dose group, 10 male and 10 female animals were treated. The 9-fold application of 2-ethylhexanol led to substance induced clinical signs like ataxia and/or abnormal position in the male animals of the 330 mg/kg and 1500 mg/kg groups and in the female animals of the 1000 mg/kg and 1500 mg/kg groups. 1 male and 4 female mice of the 1500 mg/kg dose group and 1 female mouse of the 1000 mg/kg dose group died during the study. Clinical chemistry and hematology revealed no changes that could be attributed to the test substance.
	1500 mg/kg dose group: Increase in relative stomach and liver weights in both sexes; foci in the forestomach of males and females; hyperkeratosis and focal or multifocal acanthosis and inflammatory edema in the submucosa of the forestomach as well as focal or multifocal ulceration of the mucous membrane in animals of both sexes; hypertrophy of the

membrane in animals of both sexes; hypertrophy of the hepatocytes in the liver in both sexes and focal necrosis of liver cells in one animal of both sexes; tubular giant cells in the testicular tubules in two male mice; tubular dilation and nephrosis in the renal cortex of animals that died intercurrently and centrilobular fatty infiltration in the liver of intercurrently died females.

1000 mg/kg dose group:

Increased relative liver weights in male and stomach weights in female mice; foci in the forestomach of some animals of both sexes; hyperkeratosis and focal or multifocal acanthosis and inflammatory edema in the submucosa of the forestomach as well as focal or multifocal ulceration of the mucous membrane in animals of both sexes; hypertrophy of hepatocytes in one male and one female animal; tubular dilation in the renal cortex and centrilobular fatty infiltration in the liver of the female mouse which died intercurrently.

330 mg/kg dose group:

Acanthosis in the mucous membrane of the forestomach of 2 male and 2 female mice, mostly connected with hyperkeratosis in the submucosa.

100 mg/kg dose group:

No substance-related findings.

Source

: Neste Oxo AB Stenungsund
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Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(120)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 11 Tage
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post obs. period : keine
Doses : 100; 330; 1000; 1500 mg/kg in Maisoel appliziert
Control group : yes, concurrent vehicle
NOAEL : 330 - 1000 mg/kg
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : 10 weibliche und 10 maennliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in je 5 ml/kg Maisoel appliziert.
In der 1500 mg/kg Dosisgruppe starb ein maennliches Tier waehrend der Versuchsdauer. Kein Effekt auf die Koerpergewichtsentwicklung wurde festgestellt. Bei allen maennlichen und 5 weiblichen Tieren dieser Dosisgruppe wurde Ataxie, gestraeubtes Fell, Lethargie und bei einigen Tieren Bewusstlosigkeit beschrieben. Klinisch-chemische und haematologische Untersuchungen zeigten keine Veraenderungen. Die absoluten Organengewichte vom Magen waren erhoeht, die der

	<p>Die absoluten Organgewichte vom Magen waren erhoeht, die der Hoden verringert. Auch die relativen Hodengewichte waren verringert, erhoeht waren die relativen Nieren- und Lebergewichte bei weiblichen Tieren und die relativen Magengewichte bei beiden Geschlechtern. Laesionen des Vormagens wurden bei 7 maennlichen und 2 weiblichen Tieren festgestellt.</p> <p>In der 1000 mg/kg Dosisgruppe wurden bei den maennlichen Tieren verringerte absolute und relative Hodengewichte beschrieben, keine weiteren Veraenderungen wurden festgestellt.</p> <p>In den beiden niederen Dosisgruppen wurden keine substanzbedingten Veraenderungen festgestellt.</p> <p>Der NOAEL wurde fuer die maennlichen Tiere zwischen 330 und 1000 mg/kg angegeben, fuer die weiblichen Tiere zwischen 1000 und 1500 mg/kg.</p>	
Source	: BASF AG Ludwigshafen	(121)
Species	: mouse	
Sex	: male/female	
Strain	: B6C3F1	
Route of admin.	: gavage	
Exposure period	: 11 Tage	
Frequency of treatment	: einmal taeglich, 5 Tage/Woche	
Post obs. period	: keine	
Doses	: 100; 330; 1000; 1500 mg/kg appliziert in Propylenglykol	
Control group	: yes, concurrent vehicle	
NOAEL	: 100 - 330 mg/kg	
Method	: other	
Year	:	
GLP	: yes	
Test substance	: as prescribed by 1.1 - 1.4	
Result	<p>: Je 10 weibliche und 10 maennliche Tiere wurde pro Dosis- und Kontrollgruppe eingesetzt. Die Substanz wurde in 5 ml/kg Propylenglykol appliziert.</p> <p>In der hoechsten Dosisgruppe starben 4 maennliche und 6 weibliche Tiere waehrend der Versuchsdauer. Bei den maennlichen Tiere wurde ein reduzierte Futteraufnahme, bei beiden Geschlechtern eine verminderte Wasseraufnahme festgestellt, die Koerpergewichtsentwicklung war jedoch nicht signifikant beeinflusst. Klinische Veraenderungen waren Ataxie, Lethargie, bei einigen Tieren wurde gestraeubtes Fell, Dyspnoe, Hypothermie und Bewusstlosigkeit beschrieben. Keine Veraenderungen wurden bei klinisch-chemischen und haematologischen Untersuchungen festgestellt. Die absoluten Magen- und Lebergewichte waren erhoeht, die absoluten Hodengewichte verringert. Auch die relativen Magen- und Lebergewichte waren erhoeht, wie auch die relativen Milzgewichte bei den weiblichen Tieren. Bei den maennlichen Tieren waren die relativen Hodengewichte verringert. Bei den ueberlebenden Tieren dieser Dosisgruppe wurden Laesionen im Vormagen beschrieben.</p> <p>2 Tiere der 1000 mg/kg Dosisgruppe starben waehrend der Versuchsdauer. Bei 6 maennlichen und 3 weiblichen Tieren der 1000 mg/kg Dosisgruppe wurden klinischen Veraenderungen festgestellt, diese entsprachen denen in der hoechsten Dosisgruppe. Veraenderte Organgewichte und Laesionen des Vormagens wurden auch in dieser Dosisgruppe festgestellt.</p> <p>Bei den Tieren der 330 mg/kg Dosisgruppe wurden keine</p>	

Source	<p>Bei den Tieren der 330 mg/kg Dosisgruppe wurden keine klinischen Veraenderungen festgestellt. Bei den Tieren wurden jedoch z.T. erhoehte Magen- und Lebergewichte festgestellt, auch zeigten die Tiere Laesionen im Vormagen. In der 100 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.</p> <p>: BASF AG Ludwigshafen</p>	(122)
Species	: mouse	
Sex	: male/female	
Strain	: B6C3F1	
Route of admin.	: gavage	
Exposure period	: 11 Tage	
Frequency of treatment	: einmal taeglich, 5 Tage / Woche	
Post obs. period	: keine	
Doses	: 100; 330; 1000; 1500 mg/kg in waessriger Emulsion appliziert	
Control group	: yes, concurrent vehicle	
NOAEL	: 100 - 330 mg/kg	
Method	: other	
Year	:	
GLP	: yes	
Test substance	: as prescribed by 1.1 - 1.4	
Result	<p>: Je 10 maennliche und 10 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert dem 5 ul/100 ml Cremophor EL zugesetzt wurden.</p> <p>4 weibliche und 1 maennliches Tier der 1500 mg/kg Dosisgruppe, ein weibliches Tier der 1000 mg/kg Dosisgruppe und ein maennliches Tier der Kontrollgruppe starben waehrend der Versuchsdauer.</p> <p>In der 1500 mg/kg Dosisgruppe wurde kein Effekt auf die Koerpergewichtsentwicklung festgestellt. Klinische Veraenderungen waren Ataxie, Lethargie, bei einigen Tieren gestraeubtes Fell und Bewusstlosigkeit. Klinisch-chemische und haematologische Untersuchungen zeigten keine Veraenderungen. Absolute und relative Leber- und Magengewichte waren erhoeht. Bei den meisten Tieren wurden Foci im Vormagen beschrieben. Histologisch wurde im Vormagen der Tiere Hyperkeratose, Akanthose (fokal, multifokal) und entzuendliche Oedeme der Submucosa beschrieben, bei einigen Tieren auch Ulcerationen der Schleimhaut. In der Leber wurde eine Hypertrophie der Hepatocyten, bei 2 Tieren fokale Nekrosen der Leberzellen beschrieben. Bei 2 maennlichen Tieren wurden tubulaere Riesenzellen bilateral in den testikulaeren Tubuli beobachtet. Tubulaere Dilatationen und Nephrosen der Nierenrinde wurden bei den Tieren, die waehrend des Versuchs starben festgestellt, bei einem Tier wurden auf centrilobulaer fettige Infiltrationen in der Leber festgestellt.</p> <p>Auch in der 1000 mg/kg Dosisgruppe traten die Befunde der hoechsten Dosierung bei einigen Tieren auf.</p> <p>In der 330 mg/kg Dosisgruppe wurden bei einem Tier klinische Veraenderungen (Ataxie, gestraeubtes Fell) beschrieben, auch wurden histologisch bei einigen Tieren im Vormagen Akanthose und Hyperkeratose der Schleimhaut festgestellt.</p> <p>In der 100 mg/kg Dosisgruppe wurden keine substanzbedingten Effekte festgestellt.</p>	
Source	: BASF AG Ludwigshafen	(123)

5. Toxicity

Id 104-76-7

Date 05.11.2001

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 3 Monate
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post obs. period : keine
Doses : 25; 125; 250; 500 mg/kg
Control group : yes, concurrent vehicle
NOAEL : 125 - 250 mg/kg
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Es wurden je 10 maennliche und 10 weibliche Tiere in die Versuchs- und Kontrollgruppen eingesetzt. Die Substanz wurde in 10 ml/kg Wasser appliziert, dem 5 ul/100 ml Cremophor EL zugesetzt waren. Ein Tier der 250 mg/kg Dosisgruppe starb waehrend der Versuchsdauer. In der 500 mg/kg Dosisgruppe wurden keine substanzbedingten klinischen, klinisch-chemischen und haematologischen Veraenderungen festgestellt. Das relative Magengewicht der maennlichen Tiere war erhoeht. Bei 2 maennlichen und einem weiblichen Tier wurde geringgradig Akanthose (fokal und multifokal) in der Mucosa des Vormagens beschrieben. In der 250 mg/kg Dosisgruppe wurde als einziger substanzbedingter Effekt ein erhoehtes relatives Magengewicht bei den maennlichen Tieren festgestellt. In der 25 und 125 mg/kg Dosisgruppe wurden keine Veraenderungen festgestellt.

Es wurde zusaetzliche eine Satellitenstudie mit je 3 maennlichen und weiblichen Tieren pro Dosis- und Kontrollgruppe durchgefuehrt. Bei diesen Tieren wurde am Ende der Studie das Leber- und Knochenmarkgewebe fuer elektronenmikroskopische Untersuchungen praepariert. Es wurden keine substanzbedingten Effekte festgestellt. Keine Induktion der Cyanid-resistenten Palmitoyl-CoA-Oxidase wurde festgestellt.

Source : BASF AG Ludwigshafen

(124) (125)

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : up to 5000 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative

5. Toxicity

Id 104-76-7

Date 05.11.2001

Method : other: according to Ames BN et al, Mutat Res 31, 347-364 (1975)
Year : 1975
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(126)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration : 10, 33, 100, 220 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: according to Ames BN, et al. Mut Res 31, 347-364, 1975
Year : 1975
GLP : no data
Test substance : other TS: Purity 99%
Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
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 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(127)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 0.01, 0.05, 0.25, 0.50, 1.0 ul/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: according to Ames BN, et al. Mut Res 31, 347-364, 1975.
Year : 1975
GLP : yes
Test substance : no data
Remark : Solvent:DMSO
Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(128)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 0.002-1.8 ul/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: according to Ames BN,et al. Mut Res 31, 347-364 (1975)

5. Toxicity

Id 104-76-7

Date 05.11.2001

Year : 1975
GLP : yes
Test substance : no data
Remark : Solvent: DMF
2-Ethylhexanol was tested at dose levels of 0.002 to 1.8 ul/plate. In a separate toxicity test using the TA 100 strain, 80% toxicity was observed at 1.8 ug/plate in the absence of metabolic activation. The treatment did not induce statistically significant increases in the frequency of His+ revertants.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(129)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 10, 100, 500, 1000, 5000 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : no data
Remark : Solvent: ethanol.
2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all tester strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or without activation.

Source : Neste Oxo AB Stenungsund

(130)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 4 to 2800 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : no data
Test substance : other TS: purity >97%
Remark : 2-Ethylhexanol was tested in the standard plate incorporation assay. Toxicity was observed in all tester strains at 2800 ug/plate.

Source : Neste Oxo AB Stenungsund
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Hoechst AG Frankfurt/Main
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ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(131)

5. Toxicity

Id 104-76-7
Date 05.11.2001

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538, TA 2637
Concentration : 500 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP :
Test substance :
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(132)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 1, 5, 10, 50, 100, 500, 1000 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP :
Test substance : other TS: 2-EH 98%
Remark : Solvent: DMSO

The preincubation method was used. Except for TA 1537 toxicity was observed at doses of 500 and 1000 ug/plate in all tester strains.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(133)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration :
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : no data
Test substance : other TS: purity >97%
Remark : The mutagenicity of urin from Sprague-Dawley rats dosed daily by gavage for 15 days with 2,000 mg/kg of 2-ethylhexanol was evaluated. Cultures were dosed with up to 2 ml urine using direct plating procedures.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)

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Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(134)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 10, 100, 500, 1000, 5000 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : no data
Remark : Solvent: ethanol.

2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all test strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or without activation.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(135)

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 10, 100, 500, 1000, 5000 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : no data
Remark : Solvent: ethanol.

2-Ethylhexanol was tested in the presence and absence of metabolic activation by Arochlor 1254-induced rat liver S9 fraction. Toxicity and precipitation were observed at the highest dose level in all test strains. 2-Ethylhexanol did not induce a positive response in any tester strain with or without activation.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(135)

Type : Bacterial gene mutation assay
System of testing : Salmonella typhimurium TA 100
Concentration : 0.5, 1.0, 1.5 mM
Cycotoxic conc. :
Metabolic activation : with and without
Result : positive
Method : other: as described by author
Year : 1982
GLP : no data

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Date 05.11.2001

Test substance : no data
Remark : The mutagenic activity of 2-ethylhexanol was evaluated in an 8-azaguanine resistance assay. 2-ethylhexanol was noted to be weakly mutagenic in a dose dependent way.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(136)

Type : Bacterial gene mutation assay
System of testing : Bacillus subtilis H17/M45
Concentration : 500 ug/plate
Cycotoxic conc. :
Metabolic activation :
Result : negative
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(137)

Type : Cytogenetic assay
System of testing : Chinese hamster ovary (CHO) cells
Concentration : 1.5-2.8 mM
Cycotoxic conc. :
Metabolic activation :
Result : ambiguous
Method :
Year :
GLP :
Test substance :
Remark : At 2.4 mM 2-ethylhexanol had a very slight effect on chromosomal integrity.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(138)

Type : DNA damage and repair assay
System of testing : E. coli strain W3110 (pol A+) and p3478 (pol A-)
Concentration : 10, 50, 100, 250, 500 ug/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative

5. Toxicity

Id 104-76-7

Date 05.11.2001

Method :
Year :
GLP : yes
Test substance : other TS: purity 99.7%
Remark : 2-Ethylhexanol was examined for DNA modifying activity in E. coli strain W3110 (pol A+) and its polymerase deficient derivative p3478 (pol A-). Based on a range finding study, the test article, dissolved in ethanol, was administered to cells at concentrations of 10, 50, 100, 250 and 500 ug/ml of bacterial suspension. Results were equivocal, however, as the test vehicle, ethanol, was found to be positive in the assay. The experiment was repeated using DMSO as the test vehicle and results were negative for 2-ethylhexanol.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(135)

Type : HGPRT assay
System of testing : CHO cells
Concentration : 20-400 nl/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: as described by author
Year : 1985
GLP : yes
Test substance : no data
Remark : 2-Ethylhexanol was tested at concentrations of 20 to 300 nl/ml in the absence, and 100 to 400 nl/ml in the presence of Arochlor-induced rat liver S9 fraction. Reproducible increases in mutant frequencies of CHO-cells were not observed.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(139)

Type : Mouse lymphoma assay
System of testing : L5178Y TK+/- mouse lymphoma cells
Concentration : 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18, 0.24 ul/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: as described by author
Year : 1983
GLP : yes
Test substance : other TS: purity >99.7%
Source : Neste Oxo AB Stenungsund

(140)

Type : Mouse lymphoma assay

5. Toxicity

Id 104-76-7
Date 05.11.2001

System of testing : L5178Y TK+/- mouse lymphoma cells
Concentration : 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18, 0.24 ul/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: as described by author
Year : 1983
GLP : yes
Test substance : other TS: purity >99.7%
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(128)

Type : Mouse lymphoma assay
System of testing : L5178Y TK+/- mouse lymphoma cells
Concentration : 0.018, 0.024, 0.032, 0.042, 0.056, 0.075, 0.10, 0.13, 0.18, 0.24 ul/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: as described by author
Year : 1983
GLP : yes
Test substance : other TS: purity >99.7%
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(128)

Type : Unscheduled DNA synthesis
System of testing : Primary rat hepatocytes
Concentration : 2.5, 5, 10, 25, 50, 100, 250, 500 and 1000 nl/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method :
Year :
GLP : yes
Test substance : other TS: purity > 99.7%
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(141)

Type : other: Cell transformation assay
System of testing : Balb/3T3 cells
Concentration : 0.011 to 1.5 ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: as described by author
Year : 1982
GLP : yes
Test substance :
Remark : 2-Ethylhexanol was tested in the cell transformation assay
in Balb/C-3T3 mouse embryo cells exposed to concentrations
of 1.5, 1.125, 0.75, 0.375 or 0.188 ul/ml under open vessel

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of 1.5, 1.125, 0.75, 0.375, or 0.188 ul/ml under open vessel conditions, and 0.162, 0.129, 0.043 or 0.011 ul/ml under closed vessel conditions. No statistically significant increase in transformation rates was observed at any concentration.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(142)

Type : other: Cell transformation assay
System of testing : Balb/3T3 cells
Concentration : 0.011 to 1.5.ul/ml
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: as described by author
Year : 1982
GLP : yes
Test substance :
Remark : 2-Ethylhexanol was tested in the cell transformation assay in Balb/C -3T3 mouse embryo cells exposed to concentrations of 1.5, 1.125, 0.75, 0.375, or 0.188 ul/ml under open vessel conditions, and 0.162, 0.129, 0.043 or 0.011 ul/ml under closed vessel conditions. No statistically significant increase in transformation rates was observed at any concentration.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(129)

Type : other: Cell transformation assay
System of testing : Mouse JB6 C141 cells
Concentration : 0.4 - 7.7 umol/l
Cycotoxic conc. :
Metabolic activation : without
Result : negative
Method : other: see reference
Year : 1986
GLP : no data
Test substance : no data
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(143)

Type : other: Cell transformation assay
System of testing : Balb/3T3 Clone A31 mouse embryo cells
Concentration : 30, 100 and 300 nl/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :

5. Toxicity

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Date 05.11.2001

GLP : yes
Test substance : other TS: purity > 99.7%
Source : Neste Oxo AB Stenungsund (130)

Type : other: Cell transformation assay
System of testing : Balb/3T3 Clone A31 mouse embryo cells
Concentration : 30, 100 and 300 nl/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : other TS: purity > 99.7%
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (135)

Type : other: Cell transformation assay
System of testing : Balb/3T3 Clone A31 mouse embryo cells
Concentration : 30, 100 and 300 nl/ml
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method :
Year :
GLP : yes
Test substance : other TS: purity > 99.7%
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main (135)

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

5.6 GENETIC TOXICITY 'IN VITRO'

Type : Cytogenetic assay
Species : rat
Sex : male
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 5 days
Doses : 0.02, 0.07, 0.21 ml/kg day
Result :
Method : other: as described by author
Year : 1981
GLP : yes
Test substance : other TS: purity > 99.7%
Result : Result: Groups of 5 male F-344 rats were treated with

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2-ethylhexanol. Of the 50 metaphase bone marrow cells examined from each animal, no significant increase in chromatid and chromosome breaks or structural rearrangements was noted. In addition, the mitotic index was unaffected by 2-ethylhexanol. At the dose levels tested 2-ethylhexanol did not induce detectable chromosomal aberrations after oral administration.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(144)

Type : Dominant lethal assay
Species : mouse
Sex : male
Strain : ICR
Route of admin. : oral unspecified
Exposure period : 5 days
Doses : 250, 500 and 1000 mg/kg
Result :
Method : other: as described by author
Year : 1981
GLP : yes
Test substance : other TS: purity 99.7%
Result : After treatment, each male was housed with 2 virgin females per week for 8 consecutive weeks to span the spermatogenic cycle. Females were sacrificed on day 14-17 of caging and scored for pregnancy, living fetuses and early and late fetal deaths. The fertility indices and the average number of dead and total implants per pregnancy were within the normal range. It was concluded that 2-ethylhexanol did not induce dominant lethal mutations after oral administration.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(145)

Type : Drosophila SLRL test
Species : Drosophila melanogaster
Sex : male
Strain :
Route of admin. : other: injection
Exposure period : single application
Doses : 50000 ppm
Result :
Method : other: as described by author
Year : 1985
GLP : no data
Test substance : other TS: Purity>99%
Result : 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.

Source : Neste Oxo AB Stenungsund

5. Toxicity

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(146)

Type : Drosophila SLRL test
Species : Drosophila melanogaster
Sex : male
Strain :
Route of admin. : oral feed
Exposure period : 72 hours
Doses : 20000 ppm
Result :
Method : other: as described by author
Year : 1985
GLP : no data
Test substance : other TS: 2-EH 99%
Result : Male flies were fed 2-ethylhexanol in a solution of 5% aqueous sucrose. The test substance was not mutagenic by this route.
Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(147)

Type : Drosophila SLRL test
Species : Drosophila melanogaster
Sex : male
Strain :
Route of admin. : other: injection
Exposure period : single application
Doses : 50000 ppm
Result :
Method : other: as described by author
Year : 1985
GLP : no data
Test substance : other TS: Purity>99%
Result : 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(147)

Type : Drosophila SLRL test
Species : Drosophila melanogaster
Sex : male
Strain :
Route of admin. : other: injection
Exposure period : single application
Doses : 50000 ppm
Result :
Method : other: as described by author
Year : 1985
GLP : no data
Test substance : other TS: Purity>99%
Result : 2-Ethylhexanol was tested by injection in a solution of 0.7% aqueous NaCl. There was no mutagenic effect detectable.
Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

5. Toxicity

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Date 05.11.2001

Hoechst AG Frankfurt/Main
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(147)

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : i.p.
Exposure period : single administration
Doses : 456 mg/kg
Result :
Method : other: as described by author
Year : 1982
GLP : yes
Test substance : no data
Result : B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.

Source : Neste Oxo AB Stenungsund

(148)

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : i.p.
Exposure period : single administration
Doses : 456 mg/kg
Result :
Method : other: as described by author
Year : 1982
GLP : yes
Test substance : no data
Result : B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main

(149)

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : i.p.
Exposure period : single administration
Doses : 456 mg/kg
Result :
Method : other: as described by author
Year : 1982
GLP : yes
Test substance : no data
Result : B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 30 hrs post application and 1000 PCE/animal were

5. Toxicity

Id 104-76-7

Date 05.11.2001

	harvested 30 hrs post application and 1000 PCE/animal were scored for the presence of micronuclei. 2-Ethylhexanol was not considered to be clastogenic under the conditions of this assay.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(149)
Type	: Micronucleus assay	
Species	: mouse	
Sex	: male/female	
Strain	: B6C3F1	
Route of admin.	: i.p.	
Exposure period	: two administrations	
Doses	: 456 mg/kg	
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	
Result	: B6C3F1 mice were administered 2-ethylhexanol at a dose which was equal to 80% of the LD50/7days. Bone marrow was harvested 24 hrs after the second administration (the two administrations being 24 hrs apart) and 1000 PCE/animal were scored for the presence of micronuclei. 2-ethylhexanol was not considered to be clastogenic under the conditions of this assay.	
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(149)

5.7 CARCINOGENITY

Species	: rat
Sex	: male/female
Strain	: Fischer 344
Route of admin.	: gavage
Exposure period	: 24 months
Frequency of treatment	: 5 days/week
Post. obs. period	: none
Doses	: 0, 50, 150, 500 mg/kg
Result	:
Control group	: yes, concurrent vehicle
Method	: other: according to EPA-TSCA guidelines
Year	:
GLP	: yes
Test substance	: other TS: purity 99.8%
Remark	: Vehicle: aqueous 0.005% Cremophor EL. In addition to the vehicle control groups, 50 rats/sex were dosed with water; Concurrently to the main study, a satellite study was

performed. 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 500 mg/kg. One group of rats (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 18 months and then sacrificed. Another group (50 rats/sex; recovery group) was treated with the same dose for 18 months and thereafter with vehicle only for 6 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female rats received the vehicle for 18 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.

Result : Result:

Satellite study:

In the interim sacrifice group a reduced body weight gain (both sexes) and clinical symptoms like poor general condition, labored breathing and "genital region smeared with urine" (females only) was observed. A slightly increased mortality in females was observed. The relative weight of testes and brain (males), stomach (females), liver and kidney (both sexes) were increased. In the recovery group similar effects were observed. After termination of treatment the body weight gain increased indicating a recovery effect. 18 males and 17 females died prematurely and one each had a focal hyperplasia in the forestomach. In the glandular stomach erosions were seen in 4 males and females each. Glandular cysts occurred in 6 males and 8 females.

Main study:

2-Ethylhexanol was not oncogenic in the rat under the conditions of this assay. In both sexes the sum of primary tumors, the sum of benign tumors and the sum of malignant tumors was lower in the top dose group than in either the vehicle control or the water control groups.

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(150)

Species : rat
Sex : male/female
Strain : Fischer 344
Route of admin. : gavage
Exposure period : 24 Monate
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post. obs. period : keine
Doses : 50; 150; 500 mg/kg
Result :
Control group : yes, concurrent vehicle
Method : other: EPA - TSCA oncogenicity guidelines, 798.3300
Year :
GLP : yes

Test substance	: as prescribed by 1.1 - 1.4
Result	<p>: Es wurden je 50 maennliche und 50 weibliche Tiere in die Kontroll- und Versuchsgruppen eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser appliziert, dem 5 mg/100 ml Cremophor EL zugesetzt waren.</p> <p>In der 50 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.</p> <p>150 mg/kg bewirkten eine Reduktion der Koerpergewichtsentwicklung bei den maennlichen Tieren um 16 % bei den weiblichen um 12 %. Es wurde eine leichte Zunahme der Anzahl von Tieren mit klinischen Veraenderungen (schlechter Allgemeinzustand, erschwerte Atmung, gestraeubtes Fell, Urin auf dem Fell im Genitalbereich) beschrieben.</p> <p>Bei den Tieren der 500 mg/kg Dosisgruppe wurde eine starke Reduktion der Koerpergewichtsentwicklung festgestellt (31 - 33 %). Bei den weiblichen Tieren war die Mortalitaetsrate signifikant erhoeht (58 % gegenueber 28 % in der Kontrollgruppe). Die Zahl der Tiere mit klinischen Veraenderungen war erhoeht. Bei haemotologischen Untersuchungen wurde nach 12 Monaten Behandlungsdauer bei den maennlichen Tieren eine leichte Zunahme von Anisocytose, vorwiegend Microcytose, beschrieben. Dieser Befund wurde nach 18 und 24 Monaten nicht mehr festgestellt. Pathologisch wurde bei den Tieren eine Ansteigen der Bronchopneumonien beschrieben, das in Verbindung mit der Aspiration von Mageninhalt gesehen wurde. Es wurde keine erhoehte Tumorinzidenz festgestellt, die Summe der Tumoren war geringer als in der Kontrollgruppe.</p> <p>Zur Hauptstudie wurde zusaetzlich eine Satellitenstudie mit der hoechsten Dosierung, 500 mg/kg durchgefuehrt. 2 Versuchsgruppen wurden eingesetzt, in der ersten Versuchsgruppe (10 maennliche und 10 weibliche Tiere) w urden die Tiere nach 18 Monaten getoetet und untersucht. In der 2 Versuchsgruppe (50 maennliche und 50 weibliche Tiere) wurden die Tiere 18 Monate mit der Substanz behandelt, danach 6 Monate entsprechend der Kontrolle.</p> <p>Die Futteraufnahme war bei den maennlichen Tieren, die nach 18 Monaten getoetet wurden reduziert, die Koerpergewichtsentwicklung war bei den maennlichen Tieren um 28 % bei den weiblichen um 14 % reduziert. Eine Zunahme der Tiere mit schlechtem Allgemeinzustand wurde beschrieben, die Mortalitaet der weiblichen Tiere war erhoeht. Veraenderte Organgewichte wurden beschrieben.</p> <p>Bei den Tieren, die nach 18 Monaten Behandlung eine 6-monatige Recovery-Phase hatte wurden folgende Veraenderungen beschrieben: reduzierte Futteraufnahme bei den maennlichen Tieren, die waehrend der Behandlung stark reduzierte Koerpergewichtsentwicklung war nach der Recovery-Phase weniger stark ausgepraegt. Klinischen Veraenderungen (schlechter Allgemeinzustand, erschwerte Atmung, Urin auf dem Fell in Genitalbereich) wurden festgestellt, auch die Organgewichte waren veraendert. Die Autoren sehen nur einen leichten Erholungseffekt waehrend der Recovery-Phase, aufgrund der Koerpergewichtsentwicklung.</p>
Source	: BASF AG Ludwigshafen
Species	: mouse
Sex	: male/female
Strain	: B6C3F1
Route of admin.	: gavage

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Exposure period	: 18 months
Frequency of treatment	: 5 days/week
Post. obs. period	: none
Doses	: 0, 50, 200, 750 mg/kg
Result	:
Control group	: yes, concurrent vehicle
Method	: other: according to EPA-TSCA guidelines
Year	:
GLP	: yes
Test substance	: other TS: purity 99.8%
Remark	: Vehicle: aqueous 0.005% Cremophor EL In addition to the vehicle control groups, 50 mice/sex were dosed with water. Concurrently to the main study, a satellite study was performed: 2-Ethylhexanol was administered by gavage (same vehicle as in the main study) at a dose of 750 mg/kg. One group of mice (10/sex; interim sacrifice group) was treated with 2-ethylhexanol 5 days/week over a period of 13 months and then sacrificed. Another group (50 mice/sex; recovery group) was treated with the same dose for 13 months and thereafter with vehicle only for 5 months and then sacrificed. As a control group for the interim sacrifice group 10 male and 10 female mice received the vehicle for 13 months. Control data for the recovery group were adopted from the vehicle control group and the top dose group of the parallel main study.
Result	: Result: Satellite study: The administration of 2-ethylhexanol to male and female mice for 13 months at a dose of 750 mg/kg caused increased mortality, reduced feed consumption and body weight gain in both sexes. The body weight gain of male and female animals of the recovery group were reduced as long as the animals were treated. After termination of treatment the male animals gained weight and reached nearly the values of the control group, indicating a recovery effect. No such effect was seen in females. Pathology revealed some statistically significant changes in organ weights and masses of foci in liver and stomach. One male and one female animal of the recovery group which died prematurely had a focal hyperplasia in the forestomach. Main study: 2-Ethylhexanol was not oncogenic in the mouse under the conditions of this assay. A slight increase in the incidence of hepatocellular carcinoma in the females of the high dose group was statistically significant if compared to the control group dosed with the emulsion vehicle, but not when compared to the control group dosed with water. This difference was regarded as incidental and not biologically relevant, based upon comparison with published data, and because of the lack of metastases. No statistically significant increase in tumor incidence occurred in male mice.
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main

Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(153)

Species : mouse
Sex : male/female
Strain : B6C3F1
Route of admin. : gavage
Exposure period : 18 Monate
Frequency of treatment : einmal taeglich, 5 Tage/Woche
Post. obs. period : keine
Doses : 50; 200; 750 mg/kg
Result :
Control group : yes, concurrent vehicle
Method : other: EPA-TSCA oncogenicity guidelines (798.3300)
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : Je 50 maennliche und 50 weibliche Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 10 ml/kg bidest. Wasser, dem 5 mg/100 ml Cremophor EL zugesetzt waren, appliziert.
 In der 50 und 200 mg/kg Dosisgruppe wurden keine substanzbedingten Veraenderungen festgestellt.
 In der 750 mg/kg Dosisgruppe war die Koerpergewichtsentwicklung bei den maennlichen Tieren um 26 % bei den weiblichen um 24 % reduziert, verbunden mit einer reduzierten Futteraufnahme. Die Mortalitaet war signifikant erhoeht (30 % bei beiden Geschlechtern gegenueber 4 % bei maennlichen und 8 % bei weiblichen Kontrolltieren). Bei haematologischen Untersuchungen wurde ein leichter Anstieg der polymorphkernigen Neutrophilen und eine Verminderung der Leukocyten festgestellt.
 Im Vormagen der Tiere wurde eine Zunahme der fokalen Hyperplasien des Epithels beobachtet. Bei den weiblichen Tieren wurde ein leichter Anstieg der hepatocellulaeren Carcinome festgestellt, der im Vergleich zur Kontrolle signifikant war. Im Vergleich zu historischen Kontrollen war das vermehrte Auftreten von hepatocellulaeren Carcinomen jedoch nicht signifikant, es wurden auch keine Metastasen festgestellt. Die Autoren beurteilen die Inzidenz der beobachteten Tumoren als zufaellig und ohne biologische Relevanz.
 Zur Hauptstudie wurde zusaetzliche eine Satellitenstudie durchgefuehrt. Die Tiere in der Satellitenstudie erhielten nur die hoechste Dosierung, d.h. 750 mg/kg. In der Satellitenstudie waren 3 Gruppen: eine Kontrollgruppe mit je 10 maennlichen und 10 weiblichen Tieren, eine Versuchsgruppe mit 10 weiblichen und 10 maennlichen Tieren, die Tiere dieser Gruppe wurden nach 13 Monaten Behandlung getoetet und eine weitere Versuchsgruppe mit je 50 maennlichen und 50 weiblichen Tieren, die 13 Monate behandelt wurden und danach bis zum Versuchsende (18 Monate) entsprechend der Kontrolle behandelt wurden.
 Veraenderungen bis zur Interimstoetung nach 13 Monaten waren: erhoehte Mortalitaet, reduzierte Futteraufnahme und reduzierte Koerpergewichtsentwicklung.
 In der Versuchsgruppe, in der die Tiere nach 13 Monaten Substanzbehandlung noch 5 Monate beobachtet wurden, zeigten

Substanzbehandlung noch 5 Monate beobachtete wurden, zeigten die maennlichen Tiere nach Absetzen der Behandlung eine deutliche Zunahme der Koerpergewichtsentwicklung, so dass nach 18 Monaten kein signifikanter Unterschied zu den Kontrollen festzustellen war. Bei den weiblichen Tieren wurde dieser Effekt nicht festgestellt. Bei pathologischen Untersuchungen der behandelten Tiere wurden signifikante Unterschiede bei Organgewichten festgestellt, wie auch Focibildung in der Leber und im Magen.

Source : BASF AG Ludwigshafen

(154) (155)

5.8 TOXICITY TO REPRODUCTION

Remark : No study located.
Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : gestation day 1 to 19
Frequency of treatment : daily (7 hours)
Duration of test : 20 days
Doses : 850 mg/m3
Control group : yes
Method : other: as described by author
Year : 1989
GLP : no data
Test substance : other TS: purity >99%
Result : Result: A group of Sprague-Dawley rats was exposed for 7 hours per day on gestation days 1-19 to 2-ethylhexanol at the highest concentration that could be generated as a vapour. Dams were sacrificed on day 20. 2-Ethylhexanol reduced maternal feed intake, but did not produce any malformations.
Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(156)

Species : rat

5. Toxicity

Id 104-76-7

Date 05.11.2001

Sex	: female
Strain	: Wistar
Route of admin.	: gavage
Exposure period	: gestation day 6 through 15
Frequency of treatment	: daily
Duration of test	: 20 days
Doses	: 130, 650, 1300 mg/kg day (in bidist. water containing 0.005% Cremophor EL)
Control group	: yes, concurrent vehicle
NOAEL Maternalt.	: = 130 mg/kg bw
NOAEL Teratogen	: = 650 mg/kg bw
Method	: Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	: 1987
GLP	: yes
Test substance	: other TS: purity >99.5%
Result	: Results:

2-Ethylhexanol was tested in this screening study (10 animals per dose group) for its prenatal toxicity in Wistar rats. On day 20 post coitum all surviving animals were sacrificed and assessed by gross pathology. The fetuses were dissected from the uterus, sexed, weighed and further investigated for any external, soft tissue and/or skeletal findings.

130 mg/kg dose group:
No adverse substance-related effects on dams or fetuses.

650 mg/kg dose group:
* maternal toxic effects
- 2 dams with piloerection
* embryo/fetotoxic effects
- slightly reduced mean fetal body weights
- increased frequency of fetuses with skeletal variations and retardations

1300 mg/kg dose group:
* maternal toxic effects
- markedly reduced food consumption during the whole treatment period (days 6-15 p.c.)
- distinctly reduced mean body weights (day 10 -20 p.c.)
body weight loss during days 6-10 p.c. and reduced body weight gains during days 10-15 p.c.; markedly reduced corrected body weight gain
- 6 animals found dead on days 9, 10 and 13 p.c.
- severe clinical symptoms like abdominal or lateral position, unsteady gait and apathy
- light brown-gray discoloration of the liver in the animals with intercurrent death; lung edema and emphysema in a few animals, and hemometra in 1 dam which showed vaginal hemorrhage before death
- distinctly reduced mean uterus weight
* embryo/fetotoxic effects
- increased number of resorptions and consequently markedly increased postimplantation loss
- markedly reduced mean fetal body weights
- one fetus with acaudia and atresia ani; increased incidence of fetuses with dilated renal pelvis and/or hydronephrosis
higher number of fetuses with skeletal malformations, variations and retardations.

5. Toxicity

Id 104-76-7

Date 05.11.2001

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(157)

Species : rat
Sex : female
Strain : Wistar
Route of admin. : gavage
Exposure period : single application on day 12 of gestation
Frequency of treatment : single application on day 12 of gestation
Duration of test :
Doses : 6.25, 12.5 mmol/kg (833, 1666 mg/kg)
Control group : yes, concurrent no treatment
Method : other: as described by author
Year : 1985
GLP : no data
Test substance : no data
Result : Results: The group given 833 mg/kg showed a slight increase of 2% in malformed fetuses relative to the controls (0%). The other parameters (implantation index, mean fetal weight, number of dead and resorbed fetuses) were unaffected. Simultaneous intraperitoneal administration of 150 mg caffeine / kg potentiated this effect (increase in malformed fetuses to 21.2 %). Even after a dose of 1666 mg/kg, the implantation index and percentage of dead and resorbed fetuses were unchanged, although the mean fetal body weight at 3.5 g was reduced relative to the controls (4.1 g). 22.2 % of the surviving fetuses showed malformations (controls 0%). These included hydronephrosis (7.8%), tail anomalies (4.9%), anomalies of the extremities (9.7%) and "others" (1%).

Source : Neste Oxo AB Stenungsund
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main
(158)

Species : rat
Sex : female
Strain : Wistar
Route of admin. : gavage
Exposure period : 6.- 15. Tag der Traechtigkeit
Frequency of treatment : einmal taeglich
Duration of test : bis zum 20. Tag der Traechtigkeit
Doses : 130; 650; 1300 mg/kg
Control group : yes
Method : other
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Result	: Je 10 Tiere wurden pro Versuchs- und Kontrollgruppe eingesetzt. Die Substanz wurde in 5 ml/kg bidest. Wasser appliziert, das zu 0.005 % Cremophor EL enthielt.
	Die niedrigste Dosierung hatte keine Wirkung auf die Muttertiere und Feten.
	650 mg/kg fuehrten bei 2 Muttertieren zu gestraeubtem Fell. Das Fetengewicht war leicht reduziert und die Zahl der skelettalen Variationen und Retardierungen erhoeht.
	1300 mg/kg bewirkten deutliche maternale Toxizitaet. 6 Muttertiere starben waehrend der Versuchsdauer. Die maternale Futteraufnahme war waehrend der Behandlungsdauer deutlich reduziert. Sowohl die Koerpergewichtsentwicklung wie auch das Koerpergewicht zu Versuchsende waren reduziert. Deutliche klinische Symptome traten auf. Bei den Tieren die waehrend der Behandlungsdauer starben wurden braun-graue Verfaerbungen der Leber beschrieben, Lungenoedeme und -emphyseme. Das Uterusgewicht war deutlich reduziert. Die Zahl der Resorptionen und Postimplantationsverluste war deutlich erhoeht, die Fetengewichte reduziert. Bei einem Fetus wurde Schwanzlosigkeit und Analatresie festgestellt. Die Zahl der Feten mit erweiterten Nierenbecken und Hydroureter war erhoeht, wie auch die Zahl der Feten mit skelettalen Missbildungen, Variationen und Retardierungen.
Source	: BASF AG Ludwigshafen
Species	: mouse
Sex	: female
Strain	: CD-1
Route of admin.	: gavage
Exposure period	: gestation day 7 through 14
Frequency of treatment	: daily
Duration of test	:
Doses	: 1525 mg/kg
Control group	: yes, concurrent vehicle
Method	: Chernoff-Kavlok teratogenicity screening test
Year	: 1980
GLP	: yes
Test substance	: no data
Remark	: Vehicle : corn oil.

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Observation period: until day 3 post partum.

The results of this study regarding the influence of 2-ethylhexanol on reproduction should be taken with care since the dose applied resulted in the death of more than 30 % of treated dams. Therefore, the observed effects on the offspring should be attributed to the extensive maternal toxicity and are very unlikely to be primary effects. The authors state that the results of this assay should not be used to label a chemical as teratogenic or nonteratogenic but to establish priorities for conventional testing.

Result	: This screening test was conducted with one group of 50 pregnant CD-1 mice. The dose of 1525 mg 2-ethylhexanol/kg/day was determined previously as the minimal effective dose for adult female mice. In 17 animals, test substance related mortality was observed by the end of the treatment period. Another animal died because of a dosing error. Clinical observations in dams included
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	<p>dosing error. Clinical observations in dams included languidity, ataxia, coldness to touch, wet stains, oily coat, and dark red discharge from the anus of one animal. Decreases in body weights and the reproductive index were observed in treated animals compared to controls. Decreases were also observed in the following parameters when compared to controls: mean number of live pups per litter, litter weight, pup weight on days 1 and 3, percent change in pup weight from day 1 to day 3, mean pup viability per litter from day 1 to 3, and percent of live pups per litter on day 1 post partum. The mean number and percent of dead pups in the treatment group was reported to be greater than in the control group.</p>
Source	<p>: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>
	(160)
Species	: mouse
Sex	: female
Strain	: CD-1
Route of admin.	: oral feed
Exposure period	: gestation day 0 through 17
Frequency of treatment	: daily (microencapsulated in the diet)
Duration of test	:
Doses	: 0, 17, 59, 191 mg/kg/day
Control group	: yes
NOAEL Maternalt.	: > 191 mg/kg bw
NOAEL Teratogen	: > 191 mg/kg bw
Method	: other: as described by author
Year	: 1991
GLP	: yes
Test substance	: other TS: purity >99%
Result	: Result: No dams died, delivered early or were removed from the study. Pregnancy rate was high and equivalent across all groups. There was no treatment-related maternal toxicity observed in this study.
	<p>There were no effects of exposure to dietary 2-ethylhexanol on any gestational parameters. The number of corpora lutea, uterine implantation sites, pre- and postimplantation loss, sex ratio and live fetal body weight per litter were all equivalent across all groups. There were also no treatment-related changes in the incidence of individual, external, visceral, skeletal or total malformations or variations. In conclusion, there were no maternal or developmental toxic effects of 2-ethylhexanol dietary exposure throughout gestation at any concentration tested.</p>
Source	<p>: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>

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Species	: rat
Sex	: female
Strain	: Fischer 344
Route of admin.	: dermal
Exposure period	: gestation day 6 through 15
Frequency of treatment	: daily (6 hours)
Duration of test	: 21 days
Doses	: 0.3, 1.0, 3.0 ml/kg/day (252, 840, 2520 mg/kg/day)
Control group	: yes
NOAEL Maternalt.	: = 252 - 840 mg/kg bw
NOAEL Teratogen	: > 2520 - mg/kg bw
Method	: other: according to US EPA Health Effect Guidelines
Year	: 1989
GLP	: yes
Test substance	: other TS: purity >99.7%
Result	: Result: Administration of 2-ethylhexanol by occluded cutaneous application to time-pregnant Fischer 344 rats during organogenesis at 0, 0.3, 1.0, or 3.0 ml/kg/day (25 animals per dose) resulted in maternal toxicity at 1.0 and 3.0 ml/kg/day (clinical signs of toxicity at the dosing site for both doses and reduced weight gain in the treatment period at 3.0 ml/kg/day), and no developmental toxicity at any doses tested. There was no treatment-related increased incidence of malformations at any dosage employed.
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

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5.10 OTHER RELEVANT INFORMATION

Type	: adsorption
Remark	: The percutaneous absorption rate of [14C]-2-ethylhexanol through human stratum corneum and full thickness rat skin has been measured in vitro using Franz-type glass diffusion cells. The absorption rate of 2-ethylhexanol through rat skin was 190 +-40 and 240 +-110 ug/cm2/hr in two separate studies. Similarly, the absorption rate through human stratum corneum was found to be 39 +-16 and 37 +- 10 ug/cm2/hr in two separate studies. The overall mean rate of percutaneous absorption through rat skin is 5.7 times the rate through human stratum corneum.
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main

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5. Toxicity

Id 104-76-7

Date 05.11.2001

Type	: adsorption	
Remark	: In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.	
Source	: Neste Oxo AB Stenungsund	(164)
Type	: adsorption	
Remark	: In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(164)
Type	: adsorption	
Remark	: In vitro percutaneous absorption studies were carried out for eight chemicals, including 2-ethylhexanol, using full thickness rat skin and human stratum corneum. The purpose of the studies was to compare the rates of absorption for the two species. For each of the chemicals, the observed rate using full thickness rat skin was greater than that observed for human stratum corneum.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(164)
Type	: Biochemical or cellular interactions	
Remark	: The incubation of 325.6 to 1953.5 ug/ml 2-ethylhexanol with the 9000xg supernatant of rat liver homogenate dose dependently reduced the activities of the aniline hydroxylase and the aminopyrin-N-demethylase.	
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(165)
Type	: Biochemical or cellular interactions	
Remark	: B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretrated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51	

- Source** : phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.
Neste Oxo AB Stenungsund (166)
- Type Remark** : Biochemical or cellular interactions
: The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawley rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
- Source** : Neste Oxo AB Stenungsund (167)
- Type Remark** : Biochemical or cellular interactions
: The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
- Source** : Neste Oxo AB Stenungsund (168)
- Type Remark** : Biochemical or cellular interactions
: Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the remainder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl-CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
- Source** : Neste Oxo AB Stenungsund (169)
- Type Remark** : Biochemical or cellular interactions
: Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
- Source** : Neste Oxo AB Stenungsund (170)
- Type Remark** : Biochemical or cellular interactions
: Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acetyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.
- Source** : Neste Oxo AB Stenungsund (171)
- Type** : Biochemical or cellular interactions

5. Toxicity

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Remark	: 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.	
Source	: Neste Oxo AB Stenungsund	(172)
Type Remark	: Biochemical or cellular interactions : Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentrations (3 nM), ethylhexanol also increased intracellular calcium.	
Source	: Neste Oxo AB Stenungsund	(173)
Type Remark	: Biochemical or cellular interactions : The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.	
Source	: Neste Oxo AB Stenungsund	(174)
Type Remark	: Biochemical or cellular interactions : Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O ₂ /CO ₂ -saturated buffer. Following infusion of ethylhexanol, O ₂ uptake and ketone body formation were diminished by 50 and 80%, respectively, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O ₂ -rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O ₂ tension and mitochondria are primary targets.	
Source	: Neste Oxo AB Stenungsund	(175)
Type Remark	: Biochemical or cellular interactions : 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20	

cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration preceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl_2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.

Source : Neste Oxo AB Stenungsund

(176)

Type Remark : Biochemical or cellular interactions
: 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O_2 . The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.

Source : Neste Oxo AB Stenungsund

(177)

Type Remark : Biochemical or cellular interactions
: The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanol turned out to be weak.

Source : Neste Oxo AB Stenungsund

(178)

Type Remark : Biochemical or cellular interactions
: 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activity was detected.

Source : Neste Oxo AB Stenungsund

(179)

Type Remark : Biochemical or cellular interactions
: Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).

Source : Neste Oxo AB Stenungsund

(180)

Type Remark : Biochemical or cellular interactions
: Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and

- (2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.
- Source** : Neste Oxo AB Stenungsund (99)
- Type Remark** : Biochemical or cellular interactions
: Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.
- Source** : Neste Oxo AB Stenungsund (181)
- Type Remark** : Biochemical or cellular interactions
: The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substantial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.
- Source** : Neste Oxo AB Stenungsund (182)
- Type Remark** : Biochemical or cellular interactions
: 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.
- Source** : Neste Oxo AB Stenungsund (183)
- Type Remark** : Biochemical or cellular interactions
: Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.
- Source** : Neste Oxo AB Stenungsund

(113)

Type Remark : Biochemical or cellular interactions
 : The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.

Source : Neste Oxo AB Stenungsund

(184)

Type Remark : Biochemical or cellular interactions
 : In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferation in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectable levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).

Source : Neste Oxo AB Stenungsund

(185)

Type Remark : Biochemical or cellular interactions
 : Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse hepatocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxisomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.

Source : Neste Oxo AB Stenungsund

(186)

Type Remark : Biochemical or cellular interactions
 : B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were pretreated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.

Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main

(166)

- Type Remark** :
- Biochemical or cellular interactions
 - The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawley rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.
- Source** :
- Neste Oxo AB Stenungsund
 - ECB - Existing Chemicals Ispra (VA)
 - Hoechst AG Frankfurt/Main

(167)

- Type Remark** :
- Biochemical or cellular interactions
 - The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).
- Source** :
- Neste Oxo AB Stenungsund
 - ECB - Existing Chemicals Ispra (VA)
 - Hoechst AG Frankfurt/Main

(168)

- Type Remark** :
- Biochemical or cellular interactions
 - Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the remainder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl-CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.
- Source** :
- Neste Oxo AB Stenungsund
 - ECB - Existing Chemicals Ispra (VA)
 - Hoechst AG Frankfurt/Main

(169)

- Type Remark** :
- Biochemical or cellular interactions
 - Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.
- Source** :
- Neste Oxo AB Stenungsund
 - ECB - Existing Chemicals Ispra (VA)
 - Hoechst AG Frankfurt/Main

(170)

- Type Remark** :
- Biochemical or cellular interactions
 - Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acetyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.

5. Toxicity

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Source	<p>to the control.</p> <p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(171)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(172)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentrations (3 nM), ethylhexanol also increased intracellular calcium.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(173)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(174)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O₂/CO₂-saturated buffer. Following infusion of ethylhexanol, O₂ uptake and ketone body formation were diminished by 50 and 80%, respectively, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O₂-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the</p>	

- reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O₂ tension and mitochondria are primary targets.
- Source** : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (175)
- Type Remark** : Biochemical or cellular interactions
: 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration preceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl₂ by isolated mitochondria 4 - to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.
- Source** : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (176)
- Type Remark** : Biochemical or cellular interactions
: 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O₂. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.
- Source** : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (177)
- Type Remark** : Biochemical or cellular interactions
: The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanol turned out to be weak.
- Source** : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main (178)

5. Toxicity

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Type	:	Biochemical or cellular interactions	
Remark	:	2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activity was detected.	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(179)
Type	:	Biochemical or cellular interactions	
Remark	:	Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(180)
Type	:	Biochemical or cellular interactions	
Remark	:	Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(99)
Type	:	Biochemical or cellular interactions	
Remark	:	Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.	
Source	:	Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(181)
Type	:	Biochemical or cellular interactions	
Remark	:	The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substantial increase in both wet liver weight and antipyrine	

Source	<p>substantial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.</p> <p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(182)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(183)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(113)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	(184)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferation in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectable levels of cytochrome P450 4A1 and</p>	

	immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(185)
Type Remark	: Biochemical or cellular interactions : Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse hepatocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(186)
Type Remark	: Biochemical or cellular interactions : B6C3F1 mice received a diet with 1 % di(2-ethylhexyl)-adipate for 4 weeks, followed by single gavage administration of 110 or 120 mg 14C-2-ethylhexanol per kg body weight. In the liver DNA, only trace amounts of radioactivity could be detected, which were deduced to be caused by the incorporation of metabolites of ethylhexanol. A similar result was obtained with rats. These were preterated for 4 weeks with 1% di(2-ethylhexyl)-phthalate in the diet and then received a single dose of 51 or 53 mg 14C-2-ethylhexanol /kg body weight.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(166)
Type Remark	: Biochemical or cellular interactions : The ability of 2-ethylhexanol to promote the development of putative preneoplastic lesions was evaluated. GGT+ foci were initiated in the livers of male Sprague-Dawely rats with a single dose of diethylnitrosamine following partial hepatectomy. Rats were fed a 2-ethylhexanol (0.17%) containing diet for 10 weeks. The test material produced essentially no effect with regard to number of GGT+ foci, peroxisome proliferation or liver weight.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(167)
Type Remark	: Biochemical or cellular interactions : The effect of 2-ethylhexanol on the dissociation of germinal cells from Sertoli cells in cultures of seminiferous tubule cell preparations was investigated. In contrast to	

Source	<p>cell preparations was investigated. In contrast to mono-ethylhexyl-phthalate, a concentration of 26.1 ug/ml 2-ethylhexanol did not have a detectable effect on the germinal cell dissociation (incubation time was 48 hrs).</p> <p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(168)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Rats were fed ad libitum a diet containing 2% of 2-ethylhexanol for two weeks. At the end of this period the livers were removed, pieces were taken for electron microscopy, and the remainder was homogenized and subfractioned to obtain mitochondria and microsomes. Protein and various enzyme activities were measured. 2-Ethylhexanol did not have a detectable influence on peroxisomal palmitoyl-CoA oxidation, catalase, or urate oxidase, on mitochondrial protein content, cytochrome c oxidase, carnitine-acetyl transferase, or on microsomal protein content, cytochrome P-450 and NADPH-cytochrome c reductase.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(169)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Adult rat hepatocytes cultured for 48 h in the presence of 1 mM 2-ethylhexanol contained increased numbers of peroxisomes. The peroxisome proliferation was associated with a marked increase (9-fold) in the activity of carnitine acetyltransferase.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(170)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Primary rat hepatocyte cultures were used to compare the effects of some alkylphthalate esters on peroxisomal enzyme activities and morphology. Carnitine acetyltransferase activity in hepatocytes, treated with 1 mM (=130.2 ug/ml) 2-ethylhexanol for 48 hrs, was elevated 6-fold as compared to the control.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(171)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: 2-Ethylhexanol was fed to male Swiss-Webster mice at a concentration of 2 % in the diet for 10 days. Treatment resulted in increased absolute liver weights, increased cytosolic and microsomal epoxide hydrolase and GSH S-transferase activities, and an increased cytosolic and microsomal protein content of the liver, as compared to controls.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA)</p>	

ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(172)

**Type
Remark**

- : Biochemical or cellular interactions
- : Kupffer cells, the resident hepatic macrophages, are activated by calcium and release a variety of mitogenic growth factors that may modulate cell proliferation. In this study, the cytosolic free calcium concentration in Fura-2-loaded cultured Kupffer cells was increased significantly following incubation with Wy-14,643 (1.25 mM), while equimolar concentrations of 2-ethylhexanol had no effect. However, at higher concentrations (3 nM), ethylhexanol also increased intracellular calcium.

Source

- : Neste Oxo AB Stenungsund
- ECB - Existing Chemicals Ispra (VA)
- Hoechst AG Frankfurt/Main
- Celanese GmbH Frankfurt am Main

(173)

**Type
Remark**

- : Biochemical or cellular interactions
- : The dose response relationship for peroxisome proliferation due to 2-ethylhexanol was investigated in male and female Alderley Park rats (Wistar-derived and Fischer 344) and mice (Swiss and B6C3F1). The animals were administered 2-ethylhexanol for 14 consecutive days at doses from 0 to 1.05 g/kg/day for rats and 0 to 1.75 g/kg/day for mice. At doses above 1.05 g/kg/day, 2-ethylhexanol was toxic to male and female rats, leading to death of the animals. Relative liver weights were increased in a dose-related manner in both species and sexes examined. Essentially linear dose-response relationships were observed for the induction of peroxisomal beta-oxidation (measured as palmitoyl CoA oxidation activities) in rats and mice.

Source

- : Neste Oxo AB Stenungsund
- ECB - Existing Chemicals Ispra (VA)
- Hoechst AG Frankfurt/Main
- Celanese GmbH Frankfurt am Main

(174)

**Type
Remark**

- : Biochemical or cellular interactions
- : Toxicity of 2-ethylhexanol was assessed in the perfused rat liver. Livers from starved rats were perfused with 2-ethylhexanol (3 mM) dissolved in O₂/CO₂-saturated buffer. Following infusion of ethylhexanol, O₂ uptake and ketone body formation were diminished by 50 and 80%, respectively, and cell damage, as assessed by the appearance of lactate dehydrogenase in the effluent perfusate, was apparent. Only O₂-rich upstream regions of the liver lobule were damaged as reflected by trypan blue uptake. It is concluded, that the toxicity of ethylhexanol in the liver is dependent on local O₂ tension and mitochondria are primary targets.

Source

- : Neste Oxo AB Stenungsund
- ECB - Existing Chemicals Ispra (VA)
- Hoechst AG Frankfurt/Main
- Celanese GmbH Frankfurt am Main

(175)

**Type
Remark**

- : Biochemical or cellular interactions
- : 2-Ethylhexanol (70uM) stimulated oxygen uptake in the perfused rat liver by about 10 % during the first 10 min of infusion. Perfusions with a hepatotoxic dose of ethylhexanol

	<p>infusion. Perfusions with a hepatotoxic dose of ethylhexanol (3 mM) led to a transient increase in oxygen uptake followed by a rapid inhibition of respiration of over 50 % in 10 min. Lactate dehydrogenase release, indicative of irreversible cell death, was detected in the effluent perfusate after 20 min. Within 10 min of perfusion, ethylhexanol decreased the ATP/ADP ratio from 2.5 to 0.9. Thus, marked decreases in hepatic energy state due to inhibition of respiration preceded cell death. The effect of ethylhexanol on isolated mitochondria was also studied: ethylhexanol stimulated state-4 rates of respiration, diminished coupled rates of respiration, and decreased the P/O ratio in a dose-dependent manner. It also decreased the uptake of radiolabelled CaCl_2 by isolated mitochondria 4- to 5-fold. It was hypothesized, that ethylhexanol initially uncouples oxidative phosphorylation leading to diminished ATP synthesis and collapse of ion gradients across the mitochondrial membrane.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(176)
Type Remark	<p>: Biochemical or cellular interactions : 2-Ethylhexanol causes toxicity exclusively to periportal regions of the perfused liver. To determine whether this toxicity was due to local oxygen tension or to drug delivery, isolated cylinders (plugs) of periportal and pericentral regions of the liver lobule from rats pretreated with phenobarbital were collected. Incubation of plugs with 2-ethylhexanol (0.1 to 4 mM) diminished urea synthesis in a dose-related manner and caused extensive cell damage. Plugs isolated from both regions of the liver lobule were affected similarly by ethylhexanol and O_2. The data indicate, that ethylhexanol toxicity is dependent on oxygen tension in isolated sublobular regions of the liver lobule.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(177)
Type Remark	<p>: Biochemical or cellular interactions : The in vitro inhibitory response of mouse and rat liver cytosolic glutathione S-transferase (GST) activities using the substrates 1,2-dichloro-4-nitrobenzene (DCNB) and 1,2-epoxy-3-(p-nitrophenoxy)-propane (ENPP) was determined for 2-ethylhexanol. The inhibitory effect of 2-ethylhexanol turned out to be weak.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(178)
Type Remark	<p>: Biochemical or cellular interactions : 2-Ethylhexanol was administered at 1% (w/w) in the diet to male C57BL/6 mice (details not reported). A slight increase in hepatic cytosolic (but not microsomal) epoxide hydrolase activity was detected.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main</p>	

5. Toxicity

Id 104-76-7

Date 05.11.2001

Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(179)

Type Remark : Biochemical or cellular interactions
: Up to 0.5 mM 2-ethylhexanol was added to primary rat hepatocyte cultures and the effect on peroxisomal enzyme activity was determined. Ethylhexanol had no effect on CN-insensitive palmitoyl-CoA oxidation (a peroxisomal marker).

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(180)

Type Remark : Biochemical or cellular interactions
: Male rats were fed the plasticisers di-(2-ethylhexyl)-phthalate (DEHP), di-(2-ethylhexyl)adipate (DEHA), di-(2-ethylhexyl)sebacate (DEHS), adipic acid, and diethyl-phthalate at a dietary concentration of 2 % for 3 weeks. Hepatic peroxisome proliferation in association with an increase in liver size, increase in hepatic activities of the peroxisome-associated enzymes catalase and carnitine acetyltransferase, and hypolipidemia were observed in animals treated with DEHP, DEHA, and DEHS but not in animals fed adipic acid and diethylphthalate. To relate structure to biological activity, additional groups of rats were fed 2-ethylhexanol, hexanol, 2-ethylhexanoic acid, hexanoic acid, 2-ethylhexyl-aldehyde, hexylaldehyde, and 2-ethylhexylamine at a 2 % dose level. The changes induced by 2-ethylhexanol and 2-ethylhexanoic acid were comparable to those induced by DEHP, DEHA, and DEHS.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(99)

Type Remark : Biochemical or cellular interactions
: Male F-344 rats were administered a diet containing 2 % (v/w) 2-ethylhexanol for 3 weeks. Then, serum triglyceride and cholesterol values were determined. A significant decrease in both serum cholesterol and triglyceride was found in animals treated with 2-ethylhexanol.

Source : Neste Oxo AB Stenungsund
ECB - Existing Chemicals Ispra (VA)
Hoechst AG Frankfurt/Main
Celanese GmbH Frankfurt am Main

(181)

Type Remark : Biochemical or cellular interactions
: The effects of exposure to 2-ethylhexanol on hepatic microsomal oxidation were investigated in male Sprague-Dawley rats. The metabolic clearance on antipyrine was utilized as an in vivo measure of the activity of the hepatic microsomal oxidative enzyme system. Subchronic (7 days) p.o. treatment of rats with 2-ethylhexanol produced a substantial increase in both wet liver weight and antipyrine clearance relative to corn oil-treated rats. Whereas subchronic treatment with 2-ethylhexanol produced apparent induction of hepatic microsomal oxidation enzymes, administration of a single dose was associated with

Source	<p>administration of a single dose was associated with immediate inhibition of the metabolism of antipyrine.</p> <p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(182)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: 2-Ethylhexanol was administered by gavage for 14 days to male rats (Alderly Park Wistar-derived) at a dose equivalent to 1 mmol/kg/day. This dose was selected, because administration of DEHP produced hepatocellular tumors at 6000 ppm, a dose which approximates to 1 mmol/kg/day. It could be demonstrated, that 2-ethylhexanol did not induce testicular atrophy, hepatomegaly, peroxisome proliferation or hypolipidaemia, while DEHP did produce liver effects.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(183)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Groups of six Sprague-Dawley rats were given five daily oral doses of 2.7 mmoles/kg body weight 2-ethylhexanol. No testicular damage was observed. In contrast, in animals which received corresponding oral doses of mono-(2-ethylhexyl)-phthalate the number of degenerated spermatocytes and spermatids was increased.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(113)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: The influence of several hepatotoxic chemicals, including 2-ethylhexanol, and hypoxia on phagocytic activity of Kupffer cells in perfused rat liver was investigated. A recently developed optical method was used to determine rates of phagocytosis of carbon articles by Kupffer cells in periportal and pericentral regions of the liver lobule based on changes in reflected light from the liver surface. With all chemicals studied, a rapid (10-30 min) decline in the rate of phagocytosis preceded parenchymal cell death as assessed from release of lactate dehydrogenase. These chemicals impaired parenchymal cell energy status as indicated by inhibition of oxygen uptake and bile flow prior to cell death.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(184)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: In order to investigate a proposed relationship between induction of hepatic microsomal lauric acid hydroxylase activity and peroxisome proliferation in the liver, male Wistar rats were treated with peroxisome proliferating compounds, and the lauric hydroxylase activity, the immunochemical detectable levels of cytochrome P450 4A1 and</p>	

Source	<p>immunochemical detectabel levels of cytochrome P450 4A1 and the activities of peroxisomal enzymes were determined. 2-Ethylhexanol caused an induction of levels of P450 4A1 (3-fold), lauric acid omega-hydroxylase activity (3-fold) and the activity of peroxisomal palmitoyl-CoA oxidase (2-fold).</p> <p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(185)
Type Remark	<p>: Biochemical or cellular interactions</p> <p>: Identification of the proximate peroxisome proliferator(s) derived from di-(2-ethylhexyl)-adipate has been achieved using primary hepatocyte cultures derived from different species and cyanide-insensitive fatty acetyl CoA oxidase (PCO) as a marker enzyme for peroxisome proliferation. In rat and mouse hepatocytes, the parent compound had no effect on peroxisomal beta-oxidation, but 2-ethylhexanol induced PCO activity 5-fold. No induction of peroxsomal beta-oxidation was observed in guinea pig and marmoset primary hepatocyte cultures.</p>	
Source	<p>: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(186)
Type Remark	<p>: Metabolism</p> <p>: 2-Ethylhexanol was efficiently absorbed following oral administration to rats. ¹⁴C associated with 2-ethyl[1-¹⁴C]-hexanol was rapidly excreted in respiratory CO₂ ((6-7%), faeces (8-9%) and urine (80-82%)), with essentially complete elimination by 28 h after administration.</p> <p>The amount of label recovered in CO₂ matched the amount of unlabelled 2-heptanone plus 4-heptanone recovered from urine, suggesting that both types of metabolites may have been derived from the major urinary metabolite, 2-ethylhexanoic acid, by decarboxylation following partial beta-oxidation. The ¹⁴CO₂ appeared not to be derived from acetate or by reductive decarboxylation.</p> <p>Other identified metabolites were 2-ethyl-5-hydroxyhexanoic acid, 2-ethyl-5-ketohexanoic acid, and 2-ethyl-1,6-hexenedioic acid. Only about 3% of the ethylhexanol was excreted unchanged.</p> <p>Ethylhexanol was a competitive inhibitor of yeast alcohol dehydrogenase, but a good substrate for horse alcohol dehydrogenase.</p>	
Source	<p>: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main</p>	(187)
Type Remark	<p>: Metabolism</p> <p>: From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via</p>	

	is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.	
Source	: Neste Oxo AB Stenungsund	(188)
Type	: Metabolism	
Remark	: Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.	
Source	: Neste Oxo AB Stenungsund	(189)
Type	: Metabolism	
Remark	: From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(188)
Type	: Metabolism	
Remark	: Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main	(189)
Type	: Metabolism	
Remark	: From experiments with perfused livers from starved rats it is concluded that 2-ethylhexanol is oxidized via phenobarbital-inducible pathways to metabolites which do not inhibit ketogenesis and that ethylhexanol inhibits beta-oxidation of fatty acids in mitochondria but not in peroxisomes. Treatment of rats with ethylhexanol (0.32 g/kg i.p.) decreased plasma ketone bodies from 1.6 to 0.8 mM, increased hepatic triglycerides and increased lipid predominantly in periportal regions of the liver lobule.	
Source	: Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main	(188)
Type	: Metabolism	
Remark	: Three rabbits were each given 3 ml of 2-ethylhexanol by gavage. Nearly 90% of ethylhexanol was excreted as alpha-ethylhexanoylglucuronide.	

Source : Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main (189)

Type Remark : Toxicokinetics
 : Excretion balance studies were conducted in female Fischer 344 rats with high (500 mg/kg) and low (50 mg/kg) oral doses of [14C]2-ethylhexanol, and following repeated oral dosing at the low level. Dermal exposures were conducted for 6 hrs with a 1 g/kg applied dose of [14C]2-ethylhexanol. The bioavailability of unlabeled 2-ethylhexanol at 500 mg/kg was compared following oral dosing as a neat chemical, and an emulsion in aqueous Cremophore EL. The high, low and repeated low oral doses of 2-ethylhexanol showed similar excretion balance profiles of [14C], with some evidence of metabolic saturation at the high dose. No evidence of metabolic induction was seen following the repeated low oral dosing. All of the oral doses were eliminated rapidly, predominantly in the urine during the first 24 hr following dosing. The dosing resulted in only about 5% absorption of the 1 g/kg dose, with the majority of the dose recovered unabsorbed from the dermal exposure cell at 6 hr. The majority of the oral and dermal doses were eliminated as glucuronides of oxidized metabolites of 2-ethylhexanol. The major urinary metabolites detected were glucuronides of 2-ethyladipic acid, 2-ethylhexanoic acid, and 5-hydroxy-2-ethylhexanoic acid, and 6-hydroxy-2-ethylhexanoic acid. Only trace amounts of unchanged 2-ethylhexanol were seen in urine. The bioavailability of 2-ethylhexanol, as determined by pharmacokinetic analysis of blood 2-ethylhexanoic acid levels, dosed orally as an emulsion in Cremophor EL, was found to be slightly, but not significantly, greater than 2-ethylhexanol dosed orally as a neat chemical.

Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main (190)

Type Remark : other
 : The hypotensive effect of 2-ethylhexanol was tested in rabbits and dogs. 0.002 to 0.032 mmoles/kg 2-ethylhexanol, injected i.v. into Vena jugularis or Vena femoralis, dose dependently decreased the blood pressure of rabbits. The heart rate increased considerably in direct relation to the dosage, as did the frequency of respiration. With dogs, no consistent hypotensive effects were observed.

Source : Neste Oxo AB Stenungsund
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Neste Oxo AB Stenungsund
 ECB - Existing Chemicals Ispra (VA)
 Hoechst AG Frankfurt/Main
 Celanese GmbH Frankfurt am Main

(191)

5.11 EXPERIENCE WITH HUMAN EXPOSURE

Remark	: No study located.
Source	: Neste Oxo AB Stenungsund Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Neste Oxo AB Stenungsund ECB - Existing Chemicals Ispra (VA) Hoechst AG Frankfurt/Main Celanese GmbH Frankfurt am Main
Remark	: Es liegen keine Untersuchungsberichte der BASF vor.
Source	: BASF AG Ludwigshafen

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- | | | |
|-----------|-----------|------------|
| Results: | Municipal | Industrial |
| BOD5/COD | 0.70 | 0.60 |
| BOD10/COD | 0.81 | 0.77 |
| BOD20/COD | 0.87 | 0.86 |
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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

Attachment II

I U C L I D

Data Set

Existing Chemical	: ID: 111-27-3
CAS No.	: 111-27-3
EINECS Name	: hexan-1-ol
EINECS No.	: 203-852-3
Molecular Weight	: 56.67
Molecular Formula	: C ₆ H ₁₄ O

Producer Related Part	
Company	: EUROPEAN COMMISSION- European Chemicals Bureau
Creation date	: 10.02.2000

Substance Related Part	
Company	: EUROPEAN COMMISSION- European Chemicals Bureau
Creation date	: 10.02.2000

Memo	:
------	---

Printing date	: 05.11.2001
Revision date	: 10.02.2000
Date of last Update	: 10.02.2000

Number of Pages	: 36
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Chapter (profile)	:
Reliability (profile)	:
Flags (profile)	:

1. General Information

Id 111-27-3
Date 05.11.2001

1.0.1 OECD AND COMPANY INFORMATION

Type :
Name : Givaudan Roure SA
Partner :
Date :
Street : 55, voie des Bans, BP 24
Town : 95102 Argenteuil Cedex
Country : France
Phone : 1/39 98 15 15
Telefax : 1/39 82 00 15
Telex :
Cedex :

Type :
Name : Henkel KGaA
Partner :
Date :
Street : Henkelstr. 67
Town : 40589 Duesseldorf
Country : Germany
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : Huels AG
Partner :
Date :
Street : Postfach
Town : D-45764 Marl
Country : Germany
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : NALCO-EXXON ENERGY CHEMICALS
Partner :
Date :
Street : CADLAND RD.
Town : SO45 3NP HYTHE
Country : United Kingdom
Phone : 01703 883 883
Telefax : 01703 883 882
Telex :
Cedex :

Type :
Name : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Partner :
Date :
Street : Ueberseering 40
Town : 22297 Hamburg
Country : Germany
Phone : 040-6375-0
Telefax : 040-6375-3496

1. General Information

Id 111-27-3
Date 05.11.2001

Telex : 21151320
Cedex :

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type : organic
Physical status : liquid
Purity : % w/w

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1-Hexanol
Source : Henkel KGaA Duesseldorf

1-HEXANOL (ALTSTOFF)
Source : Henkel KGaA Duesseldorf

1-Hexyl alcohol
Source : Henkel KGaA Duesseldorf

1-Hydroxyhexan
Source : Henkel KGaA Duesseldorf

1-Hydroxyhexane
Source : Henkel KGaA Duesseldorf

Alcohol C6 hexylic
Source : Givaudan Roure SA Argenteuil Cedex

Amylcarbinol
Source : Henkel KGaA Duesseldorf

Capronalkohol
Source : Henkel KGaA Duesseldorf

Caproyl alcohol
Source : Henkel KGaA Duesseldorf

Epal 108
Source : Henkel KGaA Duesseldorf

Epal 6
Source : Henkel KGaA Duesseldorf

Epal 610

1. General Information

Id 111-27-3
Date 05.11.2001

Source	: Henkel KGaA Duesseldorf
Exxal 6	
Source	: Henkel KGaA Duesseldorf
FA-C6	
Source	: Henkel KGaA Duesseldorf
Hexan-1-ol	
Source	: Henkel KGaA Duesseldorf
Hexanol	
Source	: Henkel KGaA Duesseldorf
Hexyl Alcohol	
Source	: Henkel KGaA Duesseldorf
hexyl alcohol	
Source	: Huels AG Marl
Hexyl alcohol (INCI)	
Source	: Henkel KGaA Duesseldorf
Hexyl alcohol, hexanol, C6 alcohol, hydroxyhexane, caproyl alcohol, pentylcarbinol, n-hexyl alcohol, amylcarbinol, 1-hydroxyhexane, amylcarbinol	
Source	: RWE-DEA Aktiengesellschaft für Mineralöl und Chemie Hamburg
Hexylalkohol	
Source	: Henkel KGaA Duesseldorf
n-Hexan-1-ol	
Source	: Henkel KGaA Duesseldorf
n-Hexanol	
Source	: Henkel KGaA Duesseldorf
N-Hexanol-1	
Source	: Henkel KGaA Duesseldorf
n-Hexyl alcohol	
Source	: Henkel KGaA Duesseldorf
Nansa EVM70/B	
Source	: Henkel KGaA Duesseldorf
Pentylcarbinol	
Source	: Henkel KGaA Duesseldorf

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

Production during the last 12 months :

1. General Information

Id 111-27-3
Date 05.11.2001

Import during the last 12 months :
Quantity : 10 000 - 50 000 tonnes in

1.6.1 LABELLING

Labelling : as in Directive 67/548/EEC
Symbols : Xn
Nota : C
Specific limits : yes
R-Phrases : (22) Harmful if swallowed
S-Phrases : (2) Keep out of reach of children
(24/25) Avoid contact with skin and eyes

1.6.2 CLASSIFICATION

Classification : as in Directive 67/548/EEC
Class of danger : corrosive
R-Phrases : (22) Harmful if swallowed

1.7 USE PATTERN

Type : type
Category : Non dispersive use

Type : type
Category : Wide dispersive use

Type : industrial
Category : Basic industry: basic chemicals

Type : industrial
Category : Chemical industry: used in synthesis

Type : industrial
Category : Personal and domestic use

Type : use
Category : Intermediates

Type : use
Category : Odour agents

Type : use
Category : Solvents

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAK (DE)
Limit value :
Country : Germany
Remark : not established

1. General Information

Id 111-27-3
Date 05.11.2001

Source : Huels AG Marl

(1)

1.9 SOURCE OF EXPOSURE

Remark : Industrial workers may be exposed during while handling.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 1 (weakly water polluting)
Country : Germany
Remark : No. 125 in catalogue
Source : Huels AG Marl

(1)

Classified by : KBwS (DE)
Labelled by :
Class of danger : 1 (weakly water polluting)
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

1.14.2 MAJOR ACCIDENT HAZARDS

Legislation : Störfallverordnung (DE)
Substance listed : no
No. in directive :
Country : Germany
Remark : Störfallverordnung 1991
Source : Huels AG Marl

(1)

Legislation : Störfallverordnung (DE)
Substance listed : no
No. in directive :
Remark : Not a major accident hazard.

1. General Information

Id 111-27-3
Date 05.11.2001

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

1.14.3 AIR POLLUTION

Classified by : other: VCI
Labelled by : other: VCI
Number : 3.1.7 (organic substances)
Class of danger : I
Country : Germany
Source : Huels AG Marl

(1)

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value : = -51.6 °C
Sublimation :
Method : other: not specified
Year :
GLP : no data
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(2)

2.2 BOILING POINT

Value : = 157 °C at
Decomposition :
Method : other: not specified
Year :
GLP : no data
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(3)

2.3 DENSITY

Type : density
Value : .81 - .82 g/cm³ at 20° C
Method : other: DIN 51757 B
Year :
GLP : no data
Test substance :
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(4)

Type : density
Value : .817 - .821 g/cm³ at 20° C
Method : other: DIN 51757
Year :
GLP : no
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(5)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : 1 hPa at 20° C
Decomposition :

2. Physico-Chemical Data

Id 111-27-3
Date 05.11.2001

Method
Year :
GLP : no
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(5)

Value : ca. 2 hPa at 40° C
Decomposition :
Method
Year :
GLP : no data
Test substance :
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(4)

2.5 PARTITION COEFFICIENT

Log pow : = 1.95 at ° C
Method : other (calculated): CLOGP program
Year :
GLP : no data
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(2)

2.6.1 WATER SOLUBILITY

Value : 6 g/l at 25 ° C
Qualitative : slightly soluble (0.1-100 mg/L)
Pka : at 25 ° C
PH : at and ° C
Method :
Year :
GLP : no
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(5)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : 62 ° C
Type :
Method : other: DIN 51755
Year :
GLP : no
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

2. Physico-Chemical Data

Id 111-27-3
Date 05.11.2001

Hamburg

(5)

Value : ca. 65 ° C
Type : closed cup
Method : other: DIN 51758/ISO 2719 (According to Pensky-Martens)
Year :
GLP : no data
Test substance :
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(4)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result : non flammable
Method : Directive 84/449/EEC, A.13 "Flammability (solids and liquids)"
Year :
GLP : no
Test substance :
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

2.10 EXPLOSIVE PROPERTIES

Remark : No explosive properties.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

2.11 OXIDIZING PROPERTIES

Remark : No oxidizing properties.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

2.12 ADDITIONAL REMARKS

Remark : Solidification point: ca. -50 degr. C (according to DGF-C-IV-3c).
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(4)

3. Environmental Fate and Pathways

Id 111-27-3
Date 05.11.2001

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: mixture of soil and acclimated sludge from a domestic wastewater treatment plant.
Contact time	:	
Degradation	:	ca. 58.03 % after 31 day
Result	:	other: These results indicate that the test substance is rapidly and extensively biodegraded
Deg. Product	:	
Method	:	other: modification of U.S. EPA TSCA method (40 CFR 796.3100)
Year	:	
GLP	:	no
Test substance	:	
Remark	:	From 20-24 mg of the test substance were added by weight to Teflon vial inserts which were then placed into their respective flasks. 30 ml of dichloromethane was then used to dissolve the test substance. The solvent was then evaporated leaving a film on the bottom of the flask. This was done to increase the bioavailability of the alcohol.
Source	:	RWE-DEA Aktiengesellschaft für Mineralöl und Chemie Hamburg

(6)

Type	:	aerobic
Inoculum	:	other bacteria: municipal sewage treatment plant effluent
Concentration	:	2mg/l related to Test substance related to
Contact time	:	
Degradation	:	77 % after 30 day
Result	:	readily biodegradable
Deg. Product	:	
Method	:	

3. Environmental Fate and Pathways

Id 111-27-3
Date 05.11.2001

Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : Lorol C6
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(7)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : µg/l
Analytical monitoring : yes
LC50 : 97200
Method : other: not specified
Year : 1983
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(8)

Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : µg/l
Analytical monitoring : yes
LC50 : 97700
Method : other: not specified
Year : 1984
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

Test substance : 99% purity

(9)

Type : other: not specified
Species : Alburnus alburnus (Fish, estuary)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no data
LC50 : = 120
Method : other: not specified
Year :
GLP : no data
Test substance : other TS: see remarks
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg
Test substance : The test substance was characterized as 98% pure 1 -hexanol.

(10)

Type : static
Species : Alburnus albidus costa (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : µg/l
Analytical monitoring : no
LC50 : 120000
Method : other: not specified
Year : 1979
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(11)

4. Ecotoxicity

Id 111-27-3

Date 05.11.2001

Type : static
Species : Alburnus alburnus (Fish, estuary)
Exposure period : 96 hour(s)
Unit : µg/l
Analytical monitoring : no
LC50 : 120000
Method : other: not specified
Year : 1984
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(12)

Type : static
Species : Brachydanio rerio (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : µg/l
Analytical monitoring : no
LC50 : 144000
Method : other: not specified
Year : 1982
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(13)

Type : static
Species : Leuciscus idus (Fish, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring :
LC0 : 30
LC50 : 55
LC100 : 100
Method : other: DIN 34412, part 15
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg
Test substance : Lorol C6.

(7)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : no data
EC50 : 201
Method : other: not specified
Year : 1982
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

Hamburg

(14)

Type :
 Species : Daphnia magna (Crustacea)
 Exposure period : 24 hour(s)
 Unit : mg/l
 Analytical monitoring : no
 EC50 : 240
 Method : other: not specified
 Year : 1977
 GLP : no data
 Test substance : no data
 Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
 Hamburg

(15)

Type :
 Species : Daphnia magna (Crustacea)
 Exposure period : 24 hour(s)
 Unit : mg/l
 Analytical monitoring : no
 EC0 : 152
 Method : other: not specified
 Year : 1982
 GLP : no data
 Test substance : no data
 Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
 Hamburg

(16)

Type :
 Species : Daphnia magna (Crustacea)
 Exposure period : 24 hour(s)
 Unit : mg/l
 Analytical monitoring : no
 EC100 : 270
 Method : other: not specified
 Year : 1982
 GLP : no data
 Test substance : no data
 Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
 Hamburg

(17)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Anacystis aeruginosa (Algae)
 Endpoint : growth rate
 Exposure period :
 Unit : µg/l
 Analytical monitoring : no
 LOEC : 1200
 Method : other: not specified
 Year : 1978
 GLP : no data
 Test substance : no data
 Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
 Hamburg

(18)

4. Ecotoxicity

Id 111-27-3
Date 05.11.2001

Species : Anacystis aeruginosa (Algae)
Endpoint : other: lethality
Exposure period :
Unit : µg/l
Analytical monitoring : no data
LOEC : 12000
Method : other: not specified
Year : 1978
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(19)

Species : Euglena sp. (Algae)
Endpoint : growth rate
Exposure period : 7 day
Unit : µg/l
Analytical monitoring : no data
LOEC : 75000
Method : other: not specified
Year : 1980
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(20)

Species : Scenedesmus quadricauda (Algae)
Endpoint : growth rate
Exposure period : 7 day
Unit : µg/l
Analytical monitoring : no
LOEC : 30000
Method : other: not specified
Year : 1980
GLP : no data
Test substance : no data
Remark : This is the concentration in which a 3% in extinction value
occurred.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(20)

Species : Scenedesmus quadricauda (Algae)
Endpoint : growth rate
Exposure period : 8 day
Unit : µg/l
Analytical monitoring : no
LOEC : 30000
Method : other: not specified
Year : 1978
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(21)

Species : Scenedesmus quadricauda (Algae)
Endpoint : growth rate
Exposure period :

4. Ecotoxicity

Id 111-27-3

Date 05.11.2001

Unit : µg/l
Analytical monitoring : no
EC50 : 30000
Method : other: not specified
Year : 1977
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(22)

Species : other algae: Chilomonas paramecium
Endpoint : growth rate
Exposure period : 48 hour(s)
Unit : µg/l
Analytical monitoring : no
LOEC : 18000
Method : other: not specified
Year : 1980
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(23)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 30 minute(s)
Unit : mg/l
Analytical monitoring :
EC0 : 1000
EC10 : 3000
Method : other: DIN 38412 Teil 8 (cell multiplication inhibition test)
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg
Test substance : Lorol C6.

(7)

Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 16 hour(s)
Unit : mg/l
Analytical monitoring :
EC0 : 3000
EC10 : 10000
Method : other: DIN 38412 teil 27 (respiration inhibition test)
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg
Test substance : Lorol C6.

(7)

4. Ecotoxicity

Id 111-27-3
Date 05.11.2001

Type : aquatic
Species : Tetrahymena pyriformis (Protozoa)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no data
EC50 : 300.4
Method : other: not specified
Year : 1990
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(24)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 4420 mg/kg bw
Method : other: Not specified
Year : 1977
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(25)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3210 mg/kg bw
Method : other
Year :
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(26)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3131 - 3344 mg/kg bw
Method : OECD Guide-line 401 "Acute Oral Toxicity"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(27)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 4900 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

5. Toxicity

Id 111-27-3
Date 05.11.2001

Hamburg

(28)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 4100 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(28)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 4870 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 4590 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 4000 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie

5. Toxicity

Id 111-27-3
Date 05.11.2001

RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 103 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(2)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 1950 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(2)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 1 hour(s)
Value : > 21 mg/l
Method : other
Year : 1977
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(30)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : rabbit
Strain :
Sex :

5. Toxicity

Id 111-27-3

Date 05.11.2001

Number of animals :
Vehicle :
Value : 1500 - 2000 mg/kg bw
Method : other: not specified
Year : 1977
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(31)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 2000 mg/kg bw
Method :
Year :
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(32)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 2500 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(28)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : = 3100 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(2)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :

5. Toxicity

Id 111-27-3

Date 05.11.2001

Value : = 2530 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 5000 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : i.v.
Exposure time :
Value : = 100 mg/kg bw
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

Type : other: lethality by aspiration
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Route of admin. : other: intratracheal
Exposure time :
Value : .2 other: ml per animal
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Remark : Animals were induced to aspirate the test substance by

placing 0.2 ml of the test substance into the mouth and then closing the nostrils during inspiration. 10/10 animals died immediately. The cause of death was suspected to be respiratory or cardiac arrest, or both.

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(33)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year :
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(34)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification : irritating
Method : Draize Test
Year :
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(35)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification : irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1984
GLP : yes
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(36)

Species : rabbit
Concentration :

5. Toxicity

Id 111-27-3

Date 05.11.2001

Exposure :
Exposure time :
Number of animals :
PDII :
Result : moderately irritating
EC classification :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly irritating
EC classification : irritating
Method : Draize Test
Year :
GLP : no
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(37)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : irritating
EC classification : irritating
Method : OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year : 1981
GLP : no data
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(34)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : moderately irritating
EC classification : irritating
Method : Draize Test
Year :
GLP : no

5. Toxicity

Id 111-27-3

Date 05.11.2001

Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg (38)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : moderately irritating
EC classification : irritating
Method : OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year : 1984
GLP : yes
Test substance : no data
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg (39)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly irritating
EC classification :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg (29)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : highly irritating
EC classification :
Method :
Year :
GLP : no data
Test substance :
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg
Test substance : Hexanol, 98%. (40)

5.3 SENSITIZATION

Type : Guinea pig maximization test
Species : guinea pig

5. Toxicity

Id 111-27-3

Date 05.11.2001

Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method : other: Magnusson, B. Kligman, A.M. J. Invest. Dermatol., 52, 1969.
Year : 1969
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(41)

Type : Guinea pig maximization test
Species : guinea pig
Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

Type : other: Human Maximization (as described by Epstein and Kligman)
Species : human
Number of animals :
Vehicle :
Result : not sensitizing
Classification : not sensitizing
Method : other: not specified
Year :
GLP : no data
Test substance : no data
Remark : The test substance was prepared and administered as a 1%
solution of 1-hexanol in petrolatum.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(42)

5.4 REPEATED DOSE TOXICITY

Species : rat
Sex : male/female
Strain : no data
Route of admin. : oral feed
Exposure period : 13 weeks
Frequency of treatment : food available ad lib, dietary mixture prepared weekly
Post obs. period : none
Doses : 0%, 0.25%, 0.5% and 1% (2%,4%, 6% weeks 11,12,and 13, respectively)
Control group : yes
NOAEL : > .5 %
LOAEL : = 1 %
Method : other: See Remarks
Year :

5. Toxicity

Id 111-27-3

Date 05.11.2001

GLP : no
Test substance : no data
Remark : Each test group consisted of ten males and ten females. The basal diet consisted of Purina Laboratory Chow. The compound was administered to the basal diet on a w/w basis and thoroughly mixed. Fresh diets were prepared each week. Body weights and food consumption were recorded weekly. Hematology studies and urine analyses were conducted at 30 and 90 days. Organ and body weight measurements were made on all animals from each test group at the termination of the study (13 weeks). Selected tissues were obtained from each animal and preserved for possible microscopic examination. All of the selected tissues from the control and high dosage groups were examined microscopically.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(43)

Species : dog
Sex : male/female
Strain : Beagle
Route of admin. : other: oral (dietary and capsule)
Exposure period : 13 weeks
Frequency of treatment : test diet was available ad lib, the capsule was given six days per week (high dose group)
Post obs. period : none
Doses : 0.5% (low), 1% (intermediate) and 1000 mg/kg (capsule, high dose)
Control group : other: basal diet only
NOAEL : = .5 %
LOAEL : = 1 %
Method : other: see remarks
Year :
GLP : no
Test substance : no data
Remark : The low and intermediate test groups consisted of two males and two females each. The high dose group (capsule) consisted of two males and three females. The basal diet consisted of ground Purina Dog meal. The compound was administered to the basal diet on a w/w basis and thoroughly mixed. Fresh diets were prepared each week. Body weights and feed consumption were recorded weekly. Hematological, plasma biochemistry, liver function and urine studies were performed on each dog during the pretreatment quarantine period, and at 3, 6, and 13 weeks. Organ and body weight measurements were made on all animals from each test group at the termination of the study (13 weeks). Selected tissues were obtained from each animal and preserved for possible microscopic examination. All of the selected tissues from the control and high dosage level animals were examined microscopically.

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg

(44)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium
Concentration : 8, 40, 200, 1000, and 5000 micrograms/plate
Cycotoxic conc. :

5. Toxicity

Id 111-27-3

Date 05.11.2001

Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(45)

Type : Ames test
System of testing : Salmonella typhimurium
Concentration : 6.25, 25, 100, 400, and 1600 micrograms/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471 "Genetic Toxicology: Salmonella thyphimurium Reverse Mutation Assay"
Year : 1983
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(45)

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

Species : mouse
Sex : no data
Strain : no data
Route of admin. : dermal
Exposure period : 60 weeks
Frequency of treatment : three times a week for 60 weeks
Post. obs. period : none
Doses : 20 microliters (20 grams of hexanol in 100 ml of cyclohexane)
Result :
Control group : no data specified
Method : other: not specified
Year :
GLP : no
Test substance : no data
Remark : The tumor-promoting activity of hexanol was studied on the skin of mice treated with an initiating dose of 7,12-dimethylbenz(a)anthracene, followed by the test substance. No skin tumours developed in 36 survivors.
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(42)

Species : mouse
Sex :

5. Toxicity

Id 111-27-3

Date 05.11.2001

Strain :
Route of admin. : dermal
Exposure period : 60 weeks
Frequency of treatment : 3 times a week
Post. obs. period :
Doses : 20 g in 100 ml cyclohexane
Result :
Control group :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : No tumors were observed.
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : inhalation
Exposure period : days 1-19 of gestation
Frequency of treatment : 7 hour/day
Duration of test : none
Doses : 3500 mg/m3
Control group : yes
NOAEL Maternal. : > 3500
NOAEL Teratogen : > 3500 -
Method : other: see remarks
Year : 1989
GLP : no data
Test substance : other TS
Remark : Groups of approximately 15 sprague-dawley rats were exposed to 7 h/day on gestation days 1-19 to 3500 mg/m3 1-hexanol, which was the highest concentration which could be generated as a vapor. Dams were weighed daily for the first week of exposure and weekly thereafter and were sacrificed on day 20. Fetuses were serially removed, blotted dry, examined for external malformations, sexed, weighed, fixed, and examined for visceral or skeletal defects.
Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg
Test substance : The purity of the test substance, which was described as reagent grade 1-hexanol, was >99% by gas chromatography using NIOSH analytical Method 1401.

(46)

Species : rat
Sex : female
Strain : Sprague-Dawley
Route of admin. : inhalation

5. Toxicity

Id 111-27-3

Date 05.11.2001

Exposure period : days 1-19 of gestation
Frequency of treatment : 7 hours a day
Duration of test :
Doses : max. 3500 mg/m3
Control group :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Remark : No signs of teratogenicity or embryotoxicity.
Source : Henkel KGaA.
RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

(29)

5.10 OTHER RELEVANT INFORMATION

5.11 EXPERIENCE WITH HUMAN EXPOSURE

- (1) Huels AG: Sicherheitsdatenblatt "n-Hexanol", Version 04 (inaktiv), 07.10.1997
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- (3) Registry of Toxic Effects of Chemical Substances, online search 1995.
- (4) MSDS Henkel KGaA. Lorol C 6 (DED 00003640 00, Ausgabe 01 vom 21.04.1994).
- (5) Material Safety Data Sheets, NACOL 6M, NACOL 6-97, NACOL 6-98, NACOL-99, Condea Chemie GmbH, Version 1.00.02, Int. no. 0699003, 1994.
- (6) Biodegradability of eleven VISTA ALFOL Alcohols. Technical Service Report, 6940-10-05-94, August 24, 1994.
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- (8) Veith, G.D., et.al. Estimating the Acute Toxicity of Narcotic Industrial Chemicals to Fathead Minnows. In: W.E. Bishop, R.D. Cardwell, and B.B. Heidolph (Eds.), Aquatic Toxicology and Assessment, 6th symposium, ASTM STP 802, Philadelphia, PA:90-97, 1983.
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- (15) Bringham, G. and Kuhn, G. Results of the Damaging Effect of Water Pollutants on *Daphnia Magna*. *Z. Wasser Abwasser Forsch.*, Vol. 10, No. 5, pgs. 161-166, 1977.

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- (17) Bringham, G. and Kuhn, R. Results of Toxic Action of Water Pollutants on *Daphnia magna* Straus Tested by an improved Standardized Procedure. *Z. Wasser Abwasser Forsch.*, Vol. 15, No. 1, Pgs. 106, 1982.
- (18) Bringham, G. and Kuhn, R. Testing of Substances for Their Toxicity Threshold: Model Organisms *Microcystis* (*Diplocystis*) *aeruginosa* and *Scendesmus quadricauda*. *Mit. Int. Ver. Theor. Angew. Limnol*, Vol. 21, Pgs. 275-284, 1978.
- (19) Bringham, G. and Kuhn, G. Limiting Values for the Noxious Effects of Water Pollutants to Blue Algae (*Microcystis aeruginosa* and Green Algae (*Scendesmus quadricauda*) in the . . . *Z. Vom. Wasser.*, Vol. 50, pgs. 45-60, 1978.
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6. References

Id 111-27-3
Date 05.11.2001

-
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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT

Attachment II

I U C L I D

Data Set

Existing Chemical	: ID: 112-53-8
CAS No.	: 112-53-8
EINECS Name	: dodecan-1-ol
EINECS No.	: 203-982-0
TSCA Name	: 1-Dodecanol
Molecular Formula	: C12H26O

Producer Related Part	
Company	: EUROPEAN COMMISSION- European Chemicals Bureau
Creation date	: 11.02.2000

Substance Related Part	
Company	: EUROPEAN COMMISSION- European Chemicals Bureau
Creation date	: 11.02.2000

Memo	:
------	---

Printing date	: 05.11.2001
Revision date	: 11.02.2000
Date of last Update	: 11.02.2000

Number of Pages	: 54
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Chapter (profile)	:
Reliability (profile)	:
Flags (profile)	:

1. General Information

Id 112-53-8
Date 05.11.2001

1.0.1 OECD AND COMPANY INFORMATION

Type :
Name : Aarhus Oliefabrik A/S
Partner :
Date :
Street : M.P. Bruunsgade 27
Town : 8100 Aarhus C
Country : Denmark
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : Givaudan Roure SA
Partner :
Date :
Street : 55, voie des Bans, BP 24
Town : 95102 Argenteuil Cedex
Country : France
Phone : 1/39 98 15 15
Telefax : 1/39 82 00 15
Telex :
Cedex :

Type :
Name : Henkel KGaA
Partner :
Date :
Street : Henkelstr. 67
Town : 40589 Duesseldorf
Country : Germany
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : Huels AG
Partner :
Date :
Street : Postfach
Town : D-45764 Marl
Country : Germany
Phone :
Telefax :
Telex :
Cedex :

Type :
Name : Petrasol B.V.
Partner :
Date :
Street : P.O.Box 222
Town : 4200 AE Gorinchem
Country : Netherlands
Phone : +31 183 630555
Telefax : +31 183 632272

1. General Information

Id 112-53-8
Date 05.11.2001

Telex	:	23602 petr nl
Cedex	:	
Type	:	
Name	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Partner	:	
Date	:	
Street	:	Ueberseering 40
Town	:	22297 Hamburg
Country	:	Germany
Phone	:	040-6375-0
Telefax	:	040-6375-3496
Telex	:	21151320
Cedex	:	
Type	:	
Name	:	Sidobre Sinnova
Partner	:	
Date	:	
Street	:	Allee des Platanes
Town	:	77100 Meaux
Country	:	France
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

1.0.2 LOCATION OF PRODUCTION SITE

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	% w/w

Substance type	:	organic
Physical status	:	solid
Purity	:	% w/w

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

1-Dodecanol	:	
Source	:	Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl

1. General Information

Id 112-53-8
Date 05.11.2001

1-DODECANOL (ALTSTOFF)

Source : Henkel KGaA Duesseldorf

1-Dodecyl alcohol

Source : Henkel KGaA Duesseldorf

1-Dodekanol

Source : Henkel KGaA Duesseldorf

1-Hydroxydodecan

Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Huels AG Marl

1-Hydroxydodecane

Source : Henkel KGaA Duesseldorf

Adol 10

Source : Henkel KGaA Duesseldorf

Adol 11

Source : Henkel KGaA Duesseldorf

Adol 12

Source : Henkel KGaA Duesseldorf

Alcohol C-12

Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Alcohol C12 lauric

Source : Givaudan Roure SA Argenteuil Cedex

Alfol 12

Source : Henkel KGaA Duesseldorf

ALKOHOL C12

Source : Huels AG Marl

C-12 Alcohol

Source : Henkel KGaA Duesseldorf

C12 Linear Primary Alcohol

Source : Henkel KGaA Duesseldorf

Cachalot L-50

Source : Henkel KGaA Duesseldorf

Cachalot L-90

Source : Henkel KGaA Duesseldorf

Conol 20P

Source : Henkel KGaA Duesseldorf

Dodecanol

Source : Sidobre Sinnova Meaux
Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Dodecyl alcohol

1. General Information

Id 112-53-8

Date 05.11.2001

Source	: Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Dodecyl Alcohol Source	: Henkel KGaA Duesseldorf
Dodecylalcohol Source	: Sidobre Sinnova Meaux
Dodecylalkohol Source	: Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf RWE-DEA Aktiengesellschaft für Mineralöl und Chemie Hamburg
Epal 1012 Source	: Henkel KGaA Duesseldorf
Epal 12 Source	: Henkel KGaA Duesseldorf
Epal 12/70 Source	: Henkel KGaA Duesseldorf
Epal 12/85 Source	: Henkel KGaA Duesseldorf
Epal 1214 Source	: Henkel KGaA Duesseldorf
Epal 1218 Source	: Henkel KGaA Duesseldorf
Epal 1412 Source	: Henkel KGaA Duesseldorf
Exxal 12 Source	: Henkel KGaA Duesseldorf
Hyfatol 12-70 Source	: Aarhus Oliefabrik A/S Aarhus C
Kalcohol 20 Source	: Henkel KGaA Duesseldorf
Laurex L1 Source	: Henkel KGaA Duesseldorf
Laurex NC Source	: Henkel KGaA Duesseldorf
Lauric alcohol Source	: Henkel KGaA Duesseldorf
Lauric alcohol; Dodecyl alcohol Source	: ISIS/RISKLINE, release VI, 1997, Haskoning Petrasol B.V. Gorinchem
Laurinic alcohol Source	: Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf

1. General Information

Id 112-53-8
Date 05.11.2001

	Henkel KGaA Duesseldorf Huels AG Marl
Laurol Source	: Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf
Lauryl 24 Source	: Henkel KGaA Duesseldorf
Lauryl alcohol Source	: Aarhus Oliefabrik A/S Aarhus C
Lauryl Alcohol Source	: Henkel KGaA Duesseldorf
Lauryl alcohol (INCI) Source	: Henkel KGaA Duesseldorf
Laurylalcohol Source	: Sidobre Sinnova Meaux
Laurylalkohol Source	: Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Lipocol L Source	: Henkel KGaA Duesseldorf
Lorol Source	: Henkel KGaA Duesseldorf
Lorol C 12 Source	: Henkel KGaA Duesseldorf
MA-1214 Source	: Henkel KGaA Duesseldorf
n-Dodecan-1-ol Source	: Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
n-Dodecanol Source	: Sidobre Sinnova Meaux Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
n-Dodecylalcohol Source	: Sidobre Sinnova Meaux
n-Dodecylalkohol	

1. General Information

Id 112-53-8
Date 05.11.2001

Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl
n-Dodekanol Source	:	Henkel KGaA Duesseldorf
n-Laurylalcokol Source	:	Sidobre Sinnova Meaux
n-Laurylalkohol Source	:	Henkel KGaA Duesseldorf Henkel KGaA Duesseldorf Huels AG Marl
NAA 42 Source	:	Henkel KGaA Duesseldorf
Nacol 12 Source	:	RWE-DEA Aktiengesellschaft für Mineraloel und Chemie Hamburg
Pisol Source	:	Henkel KGaA Duesseldorf
S 1298 Source	:	Henkel KGaA Duesseldorf
Sipol L 12 Source	:	Henkel KGaA Duesseldorf
Siponol 25 Source	:	Henkel KGaA Duesseldorf
Siponol L 2 Source	:	Henkel KGaA Duesseldorf
Siponol L 5 Source	:	Henkel KGaA Duesseldorf

1.3 IMPURITIES

1.4 ADDITIVES

1.5 QUANTITY

Production during the last 12 months	:	
Import during the last 12 months	:	
Quantity	:	50 000 - 100 000 tonnes in

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

Type	:	type
Category	:	Non dispersive use
Type	:	type
Category	:	Wide dispersive use
Type	:	industrial
Category	:	Chemical industry: used in synthesis
Type	:	industrial
Category	:	Metal extraction, refining and processing of metals
Type	:	industrial
Category	:	Paints, lacquers and varnishes industry
Type	:	industrial
Category	:	Personal and domestic use
Type	:	industrial
Category	:	Public domain
Type	:	industrial
Category	:	Textile processing industry
Type	:	industrial
Category	:	other: metal processing industry
Type	:	use
Category	:	Cleaning/washing agents and disinfectants
Type	:	use
Category	:	Cosmetics
Type	:	use
Category	:	Flame retardants and fire preventing agents
Type	:	use
Category	:	Hydraulic fluids and additives
Type	:	use
Category	:	Intermediates
Type	:	use
Category	:	Lubricants and additives
Type	:	use
Category	:	Odour agents
Type	:	use
Category	:	Solvents

1.7.1 TECHNOLOGY PRODUCTION/USE

1. General Information

Id 112-53-8
Date 05.11.2001

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : MAK (DE)
Limit value :
Country : Germany
Remark : MAK-Wert: not established
Source : Huels AG Marl

(1)

1.9 SOURCE OF EXPOSURE

Memo : Emissionserklaerung Huels 1992
Remark : Release into the atmosphere on production site in 1992: less than 25 kg/a
Source : Huels AG Marl

(2)

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST. HARMLESS

1.13 STATEMENTS CONCERNING WASTE

1.14.1 WATER POLLUTION

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 0 (generally not water polluting)
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(3)

Classified by : KBwS (DE)
Labelled by :
Class of danger : 0 (generally not water polluting)
Remark : German Commission for the Assessment of Water Polluting Substances (Datasheet No. 656)
Source : Transfer program
Henkel KGaA Duesseldorf

Classified by : KBwS (DE)
Labelled by : KBwS (DE)
Class of danger : 0 (generally not water polluting)
Country : Germany
Remark : KBwS-Datenblatt 656
Source : Huels AG Marl

(4) (1)

1.14.2 MAJOR ACCIDENT HAZARDS

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Legislation : Stoerfallverordnung (DE)
Substance listed : no
No. in directive :
Country : Germany
Source : Huels AG Marl

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

Source : Henkel KGaA Duesseldorf

Remark : TA Luft, Einstufung: Klasse 3 (Anhang E, Alkylalkohole)
Wassergefaehrungsklasse: WGK 0

Source : RWE-DEA Aktiengesellschaft für Mineraloel und Chemie
Hamburg

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTINGS E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value : 19 - 23 ° C
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
 Test substance : Lauryl alcohol, > = 97% purity. (5)

Value : = 23 ° C
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (6)

Value : 23.7 - 23.9 ° C
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
 Test substance : Lauryl alcohol, chem. pure, > = 99,7% was tested. (5)

Value : = 23.8 ° C
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (7)

Value : = 24 ° C
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (8)

Value : = 26 ° C
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (9)

2.2 BOILING POINT

Value : = 264.6 ° C at 1013 hPa
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (10)

Value : = 264.6 ° C at 1013 hPa
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (10)

Value : = 264.6 ° C at 1013 hPa
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (10)

Value : = 264.6 ° C at 1013 hPa
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf (10)

Value : = 264.6 ° C at 1013 hPa

2. Physico-Chemical Data

Id 112-53-8
Date 05.11.2001

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (10)

Value : = 264.6 °C at 1013 hPa
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (10)

2.3 DENSITY

Type : density
Value : = .8309 g/cm³ at 24° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (7)

Type : density
Value : .815 - .825 g/cm³ at 30° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Lauryl alcohol, > = 97% purity. (5)

Type : density
Value : = .822 g/cm³ at 40° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (6)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00022 hPa at 20° C
Decomposition :
Method : other (calculated): extrapoliert anhand Antoine-Gleichung
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (10)

Value : = .0087 hPa at 20° C
Decomposition :
Method : other (calculated): extrapoliert anhand Clausius -Clapeyronscher Gleichung
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (8)

Value : = .024 hPa at 20° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

2. Physico-Chemical Data

Id 112-53-8
Date 05.11.2001

(11)

Value : = 1.33 hPa at 91° C
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(12)

2.5 PARTITION COEFFICIENT

Log pow : = 5.06 at ° C
Method other (calculated): Methode von Nys & Rekker
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(13)

Log pow : = 5.06 at ° C
Method other (calculated): Leo, Hansch: Version CLOG P 3.3
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(14)

Log pow : = 5.13 at ° C
Method other (measured): keine weiteren Angaben
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(15)

Log pow : = 5.36 at ° C
Method other (measured): HPLC
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : ambient temperature

(14)

2.6.1 WATER SOLUBILITY

Value : = 1.69 mg/l at 16 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: measured (ueber radioaktive Markierung)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

2. Physico-Chemical Data

Id 112-53-8
Date 05.11.2001

(16)

Value : 1.9 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: measured (GC)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(17)

Value : = 2.7 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: calculated
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(18)

Value : = 2.9 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: measured (keine weiteren Angaben)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(13)

Value : = 3 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: calculated
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(19)

Value : = 4.28 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: measured (ueber Oberflaechenspannung)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(20)

2. Physico-Chemical Data

Id 112-53-8
Date 05.11.2001

Value : = 20 mg/l at 25 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: calculated
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(13)

Value : = 2.9 mg/l at 34 ° C
Qualitative :
Pka : at 25 ° C
PH : at and ° C
Method : other: measured (ueber radioaktive Markierung)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(16)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : ca. 140 ° C
Type : open cup
Method : other: DIN 51758/ISO 2719
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Lauryl alcohol, > = 97% purity.

(5)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result : non flammable
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

2.10 EXPLOSIVE PROPERTIES

Result : not explosive
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

2. Physico-Chemical Data

Id 112-53-8
Date 05.11.2001

2.11 OXIDIZING PROPERTIES

Result : no oxidizing properties
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

2.12 ADDITIONAL REMARKS

Remark : Dissoziationskonstante: $pK_a = 16.20$ (geschätzt; Methode nach Perrin, D.D. "pKa Prediction for organic acids and bases" Chapman & Hall, London, 1981) vermutlich Sekundaerzitat
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(14)

Remark : Geruch: angenehm blumenartig
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(21)

Remark : Viskositaet (40 Grad C): $9.7 \text{ mPa} \cdot \text{s}$
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(22)

Remark : Geruchsschwelle: $2.2 \pm 1.3 \text{ mg/m}^3$
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(11)

Remark : Geruchsschwelle: 0.0255 mg/l
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(23)

Remark : Geruchsschwelle: 0.0000537 mg/l
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(24)

Remark : Odor: pleasant, like nuts
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(5)

Remark : Geruch: angenehm blumenartig
Source : Henkel KGaA Duesseldorf

(21)

Remark : Viskositaet (40 Grad C): $9.7 \text{ mPa} \cdot \text{s}$
Source : Henkel KGaA Duesseldorf

(22)

Remark : Geruchsschwelle: $2.2 \pm 1.3 \text{ mg/m}^3$
Source : Henkel KGaA Duesseldorf

(11)

Remark : Geruchsschwelle: 0.0255 mg/l

2. Physico-Chemical Data

Id 112-53-8
Date 05.11.2001

Source	: Henkel KGaA Duesseldorf	(23)
Remark	: Geruchsschwelle: 0.0000537 mg/l	
Source	: Henkel KGaA Duesseldorf	(24)
Remark	: Odor: pleasant, like nuts	
Source	: Henkel KGaA Duesseldorf	(5)

3. Environmental Fate and Pathways

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3.1.1 PHOTODEGRADATION

Remark : Adsorbiert an TiO₂ wird Dodecanol (Konzentration ca. 37 mg/l) in waessriger Suspension bei Bestrahlung mit simuliertem Sonnenlicht in 2 bis 3 Stunden vollstaendig zu CO₂ und H₂O abgebaut

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(25)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic

Inoculum : other: municipal sewage treatment plant effluent

Concentration : 2mg/l related to Test substance
related to

Contact time :

Degradation : 79 % after 29 day

Result : readily biodegradable

Kinetic of test substance : 7 day = 54 %
14 day = 68 %
21 day = 80 %
%
%

Deg. Product :

Method : Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"

Year :

GLP : yes

Test substance : as prescribed by 1.1 - 1.4

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

Test condition : Nonylphenol 9.5 EO + 5 PO was used as solvent for poorly soluble test substance. Oxygen demand of solvent alone was determined and subtracted from oxygen demand of test substance plus solvent.

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(26)

Type : aerobic
Inoculum : other: sewage treatment plant effluent/biological stage
Concentration : 2mg/l related to related to
Contact time :
Degradation : 79 - 58 % after 28 day
Result : readily biodegradable
Deg. Product :
Method : Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : EG-RiLi 84/449 Anh.V C4-E
Remark : ungenügender Restsauerstoff in der höheren Prüfkonzentration
Lösungsvermittler eingesetzt
Source : Henkel KGaA Duesseldorf
Test condition : #1: 2 mg/l referring to Active Substance: 79% with parameter % BSB/CSB
#2: 5 mg/l referring to Active Substance: 58% with parameter % BSB/CSB
Test substance : Active Matter = 100 %

(27) (28)

Type : aerobic
Inoculum : activated sludge, domestic
Concentration : 100mg/l related to related to
Contact time :
Degradation : 100 % after 28 day
Result : other: readily degradable
Deg. Product :
Method : ISO Draft "BOD Test for insoluble substances"
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : two phase closed bottle test
Source : Henkel KGaA Duesseldorf
Test condition : #1: 100 mg/l referring to Chemical oxygen demand: 100% with parameter % BSB/CSB
Test substance : Active Matter = 100 %

(29) (30)

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 100mg/l related to COD (Chemical Oxygen Demand) related to
Contact time :
Degradation : 100 % after 28 day
Result :
Kinetic of test substance : 7 day = 72 %
14 day = 89 %
21 day = 93 %
%
%
Deg. Product :
Method : ISO Draft "BOD Test for insoluble substances"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

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Remark : Parameter: % BOD/COD
Source : Henkel KGaA Duesseldorf
Test condition : Direkteinwaage der Testsubstanz; kontinuierlich geschuettelt; 20 - 25 Grad C
(31)

Type : aerobic
Inoculum : predominantly domestic sewage, adapted
Contact time :
Degradation : 23.2 % after 5 day
Result :
Deg. Product :
Method : other: BOD-determination according to American Public Health Assoc. (1980), "Standard Methods for the Examination of Water and Wastewater"; 15th edition, S. 70ff.
Year : 1980
GLP :
Test substance :
Remark : Einsatzkonz.: <= 3.2 mg/l ("never exceeded the water solubility of the chemical")
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 21 +- 3 Grad C
(32) (33)

Type : aerobic
Inoculum : activated sludge, domestic, non-adapted
Concentration : 100mg/l related to COD (Chemical Oxygen Demand) related to
Contact time :
Degradation : 100 % after 28 day
Result :
Kinetic of test substance : 7 day = 72 %
14 day = 89 %
21 day = 93 %
%
%

Deg. Product :
Method : other: BOD-test for insoluble substances (BODIS-test). Closed bottle test (modification of RDA Blok test) with test substance as sole carbon source
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Parameter: % BOD/COD
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : Direkteinwaage der Testsubstanz; kontinuierlich geschuettelt; 20 - 25 Grad C
(31)

Type : aerobic
Inoculum : activated sludge, adapted
Contact time :
Degradation : 15.2 % after .3 day
Result :
Deg. Product :
Method : other: Warburg-Respirometer; method according to Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 26, 1069-1080 (1954)
Year : 1954
GLP :
Test substance :

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Remark : Einsatzkonz.: nicht angegeben
Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (34)

Type : aerobic
Inoculum : activated sludge, adapted
Contact time :
Degradation : 29.7 % after 5 day
Result :
Deg. Product :
Method : other: Warburg-Respirometer; method according to Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 26, 1069-1080 (1954)
Year : 1954
GLP :
Test substance :
Remark : Einsatzkonz.: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 20 Grad C (34)

Type : aerobic
Inoculum : domestic sewage
Contact time :
Degradation : 27 % after 5 day
Result :
Deg. Product :
Method : other: Warburg-Respirometer; method according to Bogan, R.H. & Sawyer, C.N., Sewage Ind. Wastes 26, 1069-1080 (1954)
Year : 1954
GLP :
Test substance :
Remark : Einsatzkonz.: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 20 Grad C (34)

Type : aerobic
Inoculum : other bacteria: Pseudomonas C12B
Contact time :
Degradation : ca. 100 % after 2 day
Result :
Remark : Einsatzkonz.: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 30 Grad C; geschuettelt; Messparameter: Gas-Fluessig-Chromatographie, Dodecanol als einzige C-Quelle, Wert aus Graphik ermittelt. (35)

Type :
Inoculum : other: no information
Contact time :
Degradation : 20 % after 5 day
Result :
Deg. Product :
Method : other: BOD-determination according to AFNOR-Guideline NF T90/103 (1969)
Year : 1969

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GLP :
Test substance :
Remark : Einsatzkonz.: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (36)

Type :
Inoculum : other bacteria: adapted microorganisms (no further details)
Concentration : 143mg/l related to Test substance
related to
Contact time :
Degradation : 75 % after 1 day
Result :
Deg. Product :
Method : other: BOD-determination in a Warburg-Respirometer according to Leibnitz
et al., Wasserwirtschaft-Wassertechnik 8, 410-416 (1958)
Year : 1958
GLP :
Test substance :
Remark : Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (37)

Type :
Inoculum : other: adapted microorganisms (no further details)
Concentration : 143mg/l related to Test substance
related to
Contact time :
Degradation : 75 % after 1 day
Result :
Deg. Product :
Method : other: BOD-determination in a Warburg-Respirometer according to Leibnitz
et al., Wasserwirtschaft-Wassertechnik 8, 410-416 (1958)
Year : 1958
GLP :
Test substance :
Remark : Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf (37)

Type :
Inoculum : activated sludge, non-adapted
Concentration : 500mg/l related to Test substance
related to
Contact time :
Degradation : 13.4 % after 1 day
Result :
Deg. Product :
Method : other: Warburg respirometer test
Year :
GLP :
Test substance :
Remark : Abbauversuche mit drei Belebtschlaemmen unterschiedlicher
Herkunft; Sauerstoffmangel durch Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 20 Grad C (38)

Type :

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Inoculum : other: no information
Contact time :
Degradation : 32 % after 5 day
Result :
Deg. Product :
Method : other: Warburg respirometer test
Year :
GLP :
Test substance :
Remark : Einsatzkonz.: nicht angegeben. Sauerstoffmangel durch
Oberflaechenfilm?
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(39)

Type :
Inoculum : other bacteria: Pseudomonas sp. (adapted)
Concentration : 800µmol/l related to Test substance
related to
Contact time :
Degradation : ca. 78 % after 2 day
Result :
Remark : Alkohole (C10 - C18) als Gemisch geprueft; Einzel-Abbauraten
aus GC -Peaks bestimmt; Abbau-Werte aus Graphik ermittelt
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : Inkubation in Minimalmedium mit Gemisch aus Alkoholen (C10,
C12, C14, C16 & C18) in Konzentrationen zu je 0.8 mmol/l;
geschuettelt; 30 Grad C

(40)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : flow through
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : yes
LC50 : = 1.01
Method : other: method according to US EPA Committee on Methods for Toxicity Tests with Aquatic Organisms
Year : 1975
GLP : no data
Test substance : other TS: dodecanol, no indication about purity
Remark : Toxizitaet nur auf geloesten Anteil bezogen, nicht auf Nominalkonzentration. Analyse durch Gaschromatographie.
Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
Test condition : 25 Grad C; pH 7.5; Sauerstoffsattigung > 60 %

(41) (17)

Type : flow through
Species : other: no data
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring : yes
Method :
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Result : No mortality was found at saturation concentration (1 mg/l at 20°C).
Source : Henkel KGaA Duesseldorf
Test condition : Flow-through test (5 l/h); concentration of test substance was maintained at >= 90% during test (as measured by GLC).

(42)

Type :
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
LC50 : = 1.924
Method : other: calculated (QSAR -study)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(43)

Type :
Species : Pimephales promelas (Fish, fresh water)
Exposure period :
Unit : mg/l
Analytical monitoring :
LC50 : .39 - .98
Method : other: calculated (QSAR -study)
Year :
GLP :

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Test substance :
Remark : Testdauer: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(44)

Type :
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
LC50 : = .1855
Method : other: calculated (QSAR -study; US-EPA)
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(45)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : no
EC0 : = 100
EC50 : = 320
EC100 : = 1000
Method : other: DIN 38412, Teil 11 (Bestimmung der Wirkung von Wasserinhaltsstoffen auf Kleinkrebse, Daphnia Kurzzeittest)
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Test method conforms with OECD-Guideline 202 A.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(46)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring :
EC0 : 100
EC50 : 320
EC100 : 1000
Method : other: DIN 38412, Teil 11 (Daphnia, acute toxicity test)
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : Method conforms with OECD Guide-line 202, part 1
Remark : Related to: Active Substance
Source : Henkel KGaA Duesseldorf
Test substance : Active Matter = 100 %

(47) (48)

Type :
Species : Nitocra spinipes (Crustacea)

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Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
EC50 : .8 - 1.2
Method : other: statischer Test mit Brackwasser aus der Ostsee ohne Belueftung
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : Salinitaet: 7 ppt; 20-22 Grad C; pH-Wert nicht eingestellt;
Aceton als Loesevermittler (< 0.5ml/l; EC50 (96h): 16700
mg/l)

(49) (50)

Type :
Species : Nitocra spinipes (Crustacea)
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
EC50 : = 1
Method : other: statischer Test mit Brackwasser aus der Ostsee ohne Belueftung
Year :
GLP :
Test substance :
Remark : TWEEN 80 als Loesevermittler (100 mg/l; EC50 (96h)=5000
mg/l)
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : Salinitaet: 7 ppt; 20-22 Grad C; pH-Wert nicht eingestellt;
TWEEN 80 als Loesevermittler (100 mg/l; EC50 (96h): 5000
mg/l)

(51)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Scenedesmus subspicatus (Algae)
Endpoint : growth rate
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring : no
EC0 : = .3
EC10 : = .73
EC50 : = .97
Method : other: Algen-Zellvermehrungshemmtest, DIN 38412, Teil 9
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Test method conforms with OECD-Guideline 201.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(52)

Species : Scenedesmus subspicatus (Algae)
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
EC0 : .4
EC50 : .62

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Method : other: DIN 38412, Teil 9 (Algal growth inhibition test)
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : Method conforms with OECD Guide-line 201
Remark : ErC50(0-72h) = 2,6 mg/l. Prod. wurde in unverg. Ethanol
gelöst u. die entspr. Volumina in die Testgefäße geg.. Der
Alkohol wurde vor Zugabe d. Testmed. abgedunstet.
Related to: Test substance
Source : Henkel KGaA Duesseldorf
Test substance : Active Matter = 99 %

(53) (54)

Species : Scenedesmus subspicatus (Algae)
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
EC0 : .3
EC50 : .97
EC10 : .73
Method : other: DIN 38412, Teil 9 (Algal growth inhibition test)
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : Method conforms with OECD Guide-line 201
Remark : ErC50(24-72h) > 10 mg/l. Test sollte sicherheitshalber
wiederholt werden, da ErC50 >> EbC50!
Related to: Active Substance
Source : Henkel KGaA Duesseldorf
Test substance : Active Matter = 99,7 %

(55) (56)

Species : Scenedesmus subspicatus (Algae)
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
Analytical monitoring :
EC0 : .1
EC50 : > 10
EC10 : .28
Method : other: DIN 38412, Teil 9 (Algal growth inhibition test)
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : Method conforms with OECD Guide-line 201
Remark : ErC50(0-72h) > 10 mg/l.
Related to: Test substance
Source : Henkel KGaA Duesseldorf
Test substance : Active Matter = 100 %

(57) (58)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type : aquatic
Species : Pseudomonas putida (Bacteria)
Exposure period : 30 minute(s)
Unit : mg/l
Analytical monitoring : no
EC0 : > 10000

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Method : other: DIN 38412, Teil 27 (respiration inhibition test)
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : 10 000 mg/l was highest concentration tested.
Test substance could not be completely suspended; particles remained in test solution.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : Test substance was directly weighed into test vessel, warmed to 45 degr C and treated with ultrasound for 5 minutes.
(59)

Type :
Species : Bacillus subtilis (Bacteria)
Exposure period :
Unit :
Analytical monitoring :
Remark : In gesaettigter waessriger Loesung trat gegenueber Sporen von Bacillus subtilis eine Keimungshemmung von 10 % auf. Versuchszeitraum nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; Methanol als Loesevermittler (< 0.2 M; keine Hemmung bei dieser Konz.)
(60) (61)

Type :
Species : Candida albicans (Fungi)
Exposure period : 18 hour(s)
Unit : mg/l
Analytical monitoring :
MIC : > 1000
Method : other: statischer Test
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; geschuettelt; Ethanol als Loesevermittler (keine Konzentrationsangabe; Ethanol-Kontrollen mitgelaufen)
(62)

Type :
Species : Escherichia coli (Bacteria)
Exposure period : 18 hour(s)
Unit : mg/l
Analytical monitoring :
MIC : > 1000
Method : other: statischer Test
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; geschuettelt; Ethanol als Loesevermittler (keine Konzentrationsangabe; Ethanol-Kontrollen mitgelaufen)
(62)

Type :
Species : Pseudomonas putida (Bacteria)
Exposure period : 30 minute(s)

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Unit : mg/l
Analytical monitoring :
EC0 : 10000
Method : other: DIN 38412, Teil 27 (Bacterial oxygen consumption test)
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : Method conforms with OECD Guide-line 209
Remark : LC0/EC0 entspricht der höchsten Prüfkonzentration
Related to: Test substance
Source : Henkel KGaA Duesseldorf
Test substance : Active Matter = 99 %

(63) (64)

Type :
Species : Saccharomyces cerevisiae (Fungi)
Exposure period : 72 hour(s)
Unit :
Analytical monitoring :
Remark : keine Toxizitaet bei einer Konzentration von 100 g/l
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 28 Grad C

(65)

Type :
Species : Staphylococcus aureus (Bacteria)
Exposure period : 18 hour(s)
Unit : mg/l
Analytical monitoring :
MIC : = 1000
Method : other: statischer Test
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; geschuettelt; Ethanol als Loesevermittler (keine Konzentrationsangabe; Ethanol-Kontrollen mitgelaufen)

(62)

Type :
Species : Tetrahymena pyriformis (Protozoa)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring :
EC50 : = 1.58
EC100 : = 2
NOEC : = 1.15
Method : other: photometrische Messung der Zellwachstumshemmung
Year :
GLP :
Test substance :
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(66) (67)

Type :
Species : other bacteria: Clostridium botulinum
Exposure period :
Unit : mg/l
Analytical monitoring :

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MIC : = 2.5
Method : other: static cell multiplication inhibition test according to Huhtanen, P.N., J. Milk Food Technol. 38, 762-763 (1975)
Year :
GLP :
Test substance :
Remark : Testdauer: nicht angegeben
Source : Henkel KGaA Duesseldorf
Test condition : anaerobe Bedingungen; Zellvermehrung visuell bestimmt (68)

Type :
Species : other bacteria: Clostridium botulinum
Exposure period :
Unit : mg/l
Analytical monitoring :
MIC : = 2.5
Method : other: statischer Zellvermehrungshemmtest nach Huhtanen, P.N., J. Milk Food Technol. 38, 762-763 (1975)
Year :
GLP :
Test substance :
Remark : Testdauer: nicht angegeben
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : anaerobe Bedingungen; Zellvermehrung visuell bestimmt (68)

Type :
Species : other bacteria: Mycoplasma gallisepticum
Exposure period : 144 hour(s)
Unit : mmol/l
Analytical monitoring :
NOEC : > .064
Method : other: statischer Zellvermehrungshemmtest
Year :
GLP :
Test substance :
Remark : keine Hemmung bei einer Konzentration von 0.064 mmol/l = 11.9 mg/l
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; Ethanol als Loesevermittler (< 1 % v/v, eingesetzte Konz. nicht toxisch) (69)

Type :
Species : other bacteria: Mycoplasma pneumoniae
Exposure period : 144 hour(s)
Unit : mmol/l
Analytical monitoring :
Method : other: statischer Zellvermehrungshemmtest
Year :
GLP :
Test substance :
Remark : bei einer Konzentration von 0.064 mmol/l (11.9 mg/l) 17.2 % Wachstumshemmung
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; Ethanol als Loesevermittler (< 1 % v/v, eingesetzte Konz. nicht toxisch) (69)

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Type :
Species : other bacteria: Streptococcus mutans
Exposure period : 24 hour(s)
Unit : mg/l
Analytical monitoring :
EC18 : = 2.3
Method : other: statischer Zellvermehrungshemmtest
Year :
GLP :
Test substance :
Remark : nach 4 Stunden betrug die Hemmung 26 % im Vergleich zur
unbehandelten Kontrolle
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; Ethanol als Loesevermittler (keine Konzentra-
tionsangabe, Kontrollen enthielten gleiche Menge Ethanol)

(70)

Type :
Species : other bacteria: Streptococcus mutans MT 5091
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring :
MIC : = 6.25
Method : other: statischer Zellvermehrungshemmtest
Year :
GLP :
Test substance :
Remark : MIC = minimale Hemmkonzentration
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 37 Grad C; Methanol als Loesevermittler (Konz. nicht angege-
ben, MIC nicht bestimmt);
Zellwachstum visuell als Trübung bestimmt

(71)

Type :
Species : other bacteria: mixed culture (see remarks)
Exposure period : 75 hour(s)
Unit :
Analytical monitoring :
Method : other: statischer, anaerober Test
Year :
GLP :
Test substance :
Remark : Bakterienspezies:
Mischung aus fakultativ anaeroben saeurebildenden Bakterien
(B. cereus, B. panthotenticus, B. coagulans, Ps. aeruginosa,
Lactobacillus plantarum, Corynebacterium)
bei einer Konzentration von 2.1 mg/l wurde 84 % relative
Gasproduktion, bei 20.8 mg/l 70 % relative Gasproduktion
gemessen
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test condition : 35 Grad C; zweimal taeglich geschuettelt;
Messparameter: Gasproduktion (die toxische Wirkung wurde
anhand der Reduktion der Gasproduktion gegenueber einer
unbehandelten Kontrolle festgestellt)

(72)

Type :

4. Ecotoxicity

Id 112-53-8

Date 05.11.2001

Species : other fungi: Candida 107
 Exposure period : 3 day
 Unit : g/l
 Analytical monitoring :
 EC100 : < 83
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
 Test condition : 30 Grad C; Kulturen geschuetzelt (73)

Type :
 Species : other fungi: Candida tropicalis
 Exposure period : 24 hour(s)
 Unit : g/l
 Analytical monitoring :
 EC0 : > 83
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
 Test condition : 30 Grad C; Kulturen geschuetzelt (73)

Type :
 Species : other fungi: Saccharomyces carlsbergensis
 Exposure period : 24 hour(s)
 Unit : g/l
 Analytical monitoring :
 EC100 : < 83
 Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
 Test condition : 30 Grad C; Kulturen geschuetzelt (73)

Type :
 Species : other fungi: see remarks
 Exposure period :
 Unit :
 Analytical monitoring :
 Method : other: test for inhibition of spore germination
 Year :
 GLP :
 Test substance :
 Remark : Species: no antifungal activity up to:

Aspergillus niger 10000 mg/l (5 d; 28 degr. C; pH 5.6)
 Trichoderma viride 100 mg/l (")
 Trichophyton
 mentagrophytes * (")
 Myroecium verrucaria * (")
 Candida albican 100 mg/l (20 h; 37 degr. C; pH 5.6)
 Mucor mucedo 1000 mg/l (")

* antifungal activity at all concentrations tested (lowest tested concentration: 100 mg/l).

Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
 Test condition : petri dishes with Sabouraud agar containing test substance were inoculated with 1 drop of spore suspension (6 x 10 exp 6 spores/ml). Test substance was dissolved in dimethyl sulfoxide (no particulars on end concentration in test). Tested concentrations: 100, 1000 and 10000 mg/l. (74)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 21 day
Unit : mg/l
Analytical monitoring : no
NOEC : = 1
LCEC : = 3
Method : other: according to UBA-Verfahrensvorschlag: "Verlaengerter Toxizitaetstest bei Daphnia magna" (Stand: 1.2.1984)
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Remark : Most sensitive parameter: number of offspring/parent.
 Test method conforms with OECD-Guideline 202, Part 2.
Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(75)

Species : Daphnia magna (Crustacea)
Endpoint :
Exposure period : 21 day
Unit : mg/l
Analytical monitoring :
NOEC : 1
LCEC : 3
Method : other: Daphnia-Life-Cycle-Test (UBA-Proposition February 1984)
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4
Method : Method conforms with OECD Guide-line 202, part 2.
 Verlaengerter Toxizitaetstest bei Daphnia magna. Bestimmung der NOEC fuer Reproduktionsrate, Mortalitaet und den Zeitpunkt des ersten Auftretens von Nachkommen).
 UBA-Verfahrensvorschlag vom Februar...
Remark : Related to: Active Substance
Source : Henkel KGaA Duesseldorf
Test substance : Active Matter = 100 %

(76) (77)

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

Species : other terrestrial plant: Pinus strobus
Endpoint :
Exposure period :
Unit :
Remark : Dodecanol stimuliert die Keimung von Pollen der Pinie (Pinus strobus) in Konzentrationen bis 25 ul/l; bei 50 und 100 ul/l wird die Keimung leicht gehemmt.
Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(78)

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

Remark : Mueckentoxizitaet:
 LD50 = 0.04 l/m2 (Eier von Aedes aegypti, 72 h)
 LD90 = 0.07 l/m2 (Eier von Aedes aegypti, 72 h)
 LD50 = 0.04 l/m2 (Eier von Aedes scutellaris, 72 h)
 LD90 = 0.07 l/m2 (Eier von Aedes scutellaris, 72 h)
 vergleichbare Werte bei Larven und Puppen
 Angaben in l/m2 Wasseroberflaeche; 150 ml/Testansatz; T =
 25-27 Grad C; 0.04 l/m2 = 1360 mg/l; 0.07 l/m2 = 2380 mg/l

Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(79)

Remark : Mueckentoxizitaet:
 Abtoetung aller eingesetzten Larven und Puppen von Culex
 quinquefasciatus in einem Versuchszeitraum von 48 h bei
 einer Konzentration von ca. 2.9 mg/l; T = 25 Grad C

Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(80)

Remark : Assimilation durch Mikroorganismen:
 Der Pseudomonas-Stamm C12B kann auf Dodecanol als einziger
 Kohlenstoffquelle wachsen.

Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(81)

Remark : Virentoxizitaet:
 30 min. Inkubation mit Testsubstanz bei Raumtemperatur;
 Parameter: Reduktion der plaque-forming units.
 Bacteriophage phi 6: EC50 = 0.007 mM (= 1.3 mg/l)
 Bacteriophage phi 23-1-a: EC50 = > 1 mM (> 186.3 mg/l)

Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(82)

Remark : Mit Dodecanol getraenkte Filterplaettchen hemmen das Wachs-
 tum von Pilzen (Candida albicans, Trichophyton mentagro-
 phytes und rubrum, Epidermophyton floccosum) und in
 geringerem Ausmass von gram-negativen Bakterien (Pseudomonas
 aeruginosa, Escherichia coli). Keine Hemmung von gram-
 positiven Bakterien (Bacillus subtilis, Staphylococcus
 aureus).

Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(83)

Remark : Toxizitaet gegenueber Kaulquappen (*Rana temporaria*):
Dodecanol narkotisiert Kaulquappen von *Rana temporaria* ab
einer Konzentration von 0.0075 mM = 1.4 mg/l (Parameter:
Reflexbewegungen nach mechanischem Stimulus). Narkose ist
reversibel.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(84)

Remark : Toxizitaet gegenueber Kaulquappen (Spezies nicht angegeben):
EC50 = 5.4 uM (1 mg/l). Parameter: Verlust des Gleichge-
wichtssinnes. Effekte sind reversibel.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(85)

Remark : Mueckentoxizitaet:
Abtoetung aller eingesetzten Larven und Puppen von *Culex*
quinquefasciatus in einem Versuchszeitraum von 48 h bei
einer Konzentration von ca. 2.9 mg/l; T = 25 Grad C

Source : Henkel KGaA Duesseldorf

(80)

Remark : Assimilation durch Mikroorganismen:
Der *Pseudomonas*-Stamm C12B kann auf Dodecanol als einziger
Kohlenstoffquelle wachsen.

Source : Henkel KGaA Duesseldorf

(81)

Remark : Virentoxizitaet:
30 min. Inkubation mit Testsubstanz bei Raumtemperatur;
Parameter: Reduktion der plaque-forming units.

Bacteriophage phi 6: EC50 = 0.007 mM (= 1.3 mg/l)
Bacteriophage phi 23-1-a: EC50 = > 1 mM (> 186.3 mg/l)

Source : Henkel KGaA Duesseldorf

(82)

Remark : Mit Dodecanol getraenkte Filterplaettchen hemmen das Wachs-
tum von Pilzen (*Candida albicans*, *Trichophyton mentagro-
phytes* und *rubrum*, *Epidermophyton floccosum*) und in
geringerem Ausmass von gram-negativen Bakterien (*Pseudomonas*
aeruginosa, *Escherichia coli*). Keine Hemmung von gram-
positiven Bakterien (*Bacillus subtilis*, *Staphylococcus*
aureus).

Source : Henkel KGaA Duesseldorf

(83)

Remark : Toxizitaet gegenueber Kaulquappen (*Rana temporaria*):
Dodecanol narkotisiert Kaulquappen von *Rana temporaria* ab
einer Konzentration von 0.0075 mM = 1.4 mg/l (Parameter:
Reflexbewegungen nach mechanischem Stimulus). Narkose ist
reversibel.

Source : Henkel KGaA Duesseldorf

(84)

Remark : Toxizitaet gegenueber Kaulquappen (Spezies nicht angegeben):
EC50 = 5.4 uM (1 mg/l). Parameter: Verlust des Gleichge-
wichtssinnes. Effekte sind reversibel.

Source : Henkel KGaA Duesseldorf

(85)

5. Toxicity

Id 112-53-8
Date 05.11.2001

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 5000 mg/kg bw
Method : other: Henkel-method "Acute oral toxicity"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Limit-Test
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(86)

Type : LD50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 5000 mg/kg bw
Method : OECD Guide-line 401 "Acute Oral Toxicity"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : Limit-Test
Source : Henkel KGaA Duesseldorf

(87)

Type : LD50
Species : mouse
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 3125 mg/kg bw
Method : Directive 84/449/EEC, B.1 "Acute toxicity (oral)"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA Duesseldorf

(88)

Type : LD50
Species : rabbit
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 30000 mg/kg bw
Method : other: not specified
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Calculated from the dose originally given (36 ml/kg) and the

density (0.83).
Seven rabbits which survived a dose of 36 ml technical lauryl alcohol/kg body weight, demonstrated no significant gross or microscopic organ injury.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(89)

5.1.2 ACUTE INHALATION TOXICITY

Type : LC0
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time : 18 hour(s)
Value : ca. 1 mg/l
Method : other: chamber
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : No deaths occurred in any of the exposed animals.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(90)

Type : LC50
Species : rat
Strain :
Sex :
Number of animals :
Vehicle :
Exposure time :
Method : other
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Ten animals were exposed by aspiration to ca. 600 mg/kg dodecanol, and were observed for max. 24 h prior to sacrifice. Nine rats died during the observation period, seven deaths occurring within 7-30 minutes. Cause of death reported as massive, extensive, severe pulmonary haemorrhage.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(91)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Species : guinea pig
Strain :
Sex :
Number of animals :
Vehicle :
Value : > 8300 mg/kg bw
Method : other: not specified

5. Toxicity

Id 112-53-8

Date 05.11.2001

Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Calculated from the dose originally given (10 ml/kg) and the density (0.83).
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(89)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : highly irritating
EC classification :
Method : Draize Test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Fifty percent lauryl alcohol was tested. The exposure time was 24 hours under occlusion.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(92)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : irritating
EC classification :
Method : other: Henkel-method "Acute skin irritation"
Year : 1977
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : 1-Dodecanol was applied in a concentration of 50% in vaseline.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(92)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : slightly irritating
EC classification :
Method : Directive 84/449/EEC, B.4 "Acute toxicity (skin irritation)"

5. Toxicity

Id 112-53-8
Date 05.11.2001

Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA Duesseldorf (88)

Species : guinea pig
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : not irritating
EC classification :
Method : other: patch test, semi-occlusive
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : 1-Dodecanol was tested 50% in vaseline for 24 h. No skin irritation was observed.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (92)

Species : human
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : not irritating
EC classification :
Method : other: see Remarks
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Volunteers; 50 %ig; 24 h Contact time; occlusive
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf (92)

Species : human
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : not irritating
EC classification : not irritating
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1984
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA Duesseldorf (93)

Species : other: hairless mouse
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :

5. Toxicity

Id 112-53-8

Date 05.11.2001

Result : not irritating
EC classification :
Method : other: Henkel KGaA "Skin irritation in hairless mice"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : The substance was applied once.
Source : Henkel KGaA Duesseldorf

(88)

Species : other: hairless mouse
Concentration :
Exposure :
Exposure time :
Number of animals :
PDII :
Result : slightly irritating
EC classification :
Method : other: Henkel KGaA "Skin irritation in hairless mice"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : The substance was applied twice daily to the same area of skin and gently massaged into it.
Source : Henkel KGaA Duesseldorf

(88)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : slightly irritating
EC classification :
Method : other: not specified
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : Three rabbits were dosed with 0.1 ml/unwashed of undiluted commercial Lauryl alcohol. Maximum average irritation scores were 9.3 at 1 h. Most scores returned to zero within 3-4 days, but in one animal 14 day were required.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(94)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : slightly irritating
EC classification :
Method : Draize Test
Year : 1959
GLP : no

5. Toxicity

Id 112-53-8

Date 05.11.2001

Test substance : other TS
Remark : The tested Dodecanol/Tetradecanol mixture exerts only very mild irritating effects on the eyes of rabbits that normally wouldn't justify a classification as "irritant to the eye".
With respect to the fact that some fatty alcohols are irritating to the skin as well as irritating to the eye, Henkel has decided to label the C10-C14 fatty alcohols consistently with the R-phrases R 36/38.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Analogy! The product "Lorol spezial-Type 70" was tested. This product consists of 70% C12- and 30% C14-fatty alcohols.

(95)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : slightly irritating
EC classification : not irritating
Method : Draize Test
Year :
GLP : no data
Test substance : other TS
Remark : Maximum average irritation scores were 9.3 at 1 h. Most scores returned to zero within 3-4 days, but in one animal 14 day were required.
Source : Henkel KGaA Duesseldorf
Test substance : Analogy to Alcohols C12-14 (80206-82-2), containing 63-68 % C12- and 24-25 % C14-alcohol

(96)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : slightly irritating
EC classification :
Method : Draize Test
Year : 1959
GLP : no
Test substance : other TS
Remark : The tested Dodecanol/Tetradecanol mixture exerts only very mild irritating effects on the eyes of rabbits.
Source : Henkel KGaA Duesseldorf
Test substance : Analogy! The product "Lorol spezial-Type 70" was tested. This product consists of 70% C12- and 30% C14-fatty alcohols.

(97)

Species : rabbit
Concentration :
Dose :
Exposure Time :
Comment :
Number of animals :
Result : slightly irritating

5. Toxicity

Id 112-53-8

Date 05.11.2001

EC classification :
Method : Draize Test
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA Duesseldorf

(88)

5.3 SENSITIZATION

Type : other: maximation test
Species : human
Number of animals :
Vehicle :
Result : not sensitizing
Classification :
Method : other: method not specified
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Remark : A maximation test was carried out on 25 volunteers using a 4 % concentration of lauryl alcohol in petrolatum. No case of sensitization was reported.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : See remark.

(98)

5.4 REPEATED DOSE TOXICITY

Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : oral feed
Exposure period : 37 days
Frequency of treatment : permanent by diet
Post obs. period :
Doses : 0, 100, 500, 2000 mg/kg bw/day
Control group : yes
NOAEL : = 100 mg/kg bw
Method : other: OECD Combined Repeat dose and Reproductive/Developmental Toxicity Screening Test.
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : The NOEL given is for the reduction in mean white blood cell count. Further, some changes were observed in plasma free cholesterol. No other effects were seen in the macroscopic and histological examinations. The NOAEL may therefore be greater than 100 mg/kg bw/day.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : 99% Dodecanol from Sigma (# L 5375) was tested.

(99)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test
System of testing : Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537, TA 1538
Concentration : 4, 20, 100, 500 and 2.500 ug per plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Henkel-method "Salmonella typhimurium reverse mutation assay"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : The test sample was suspended in water using Tween 80 as surfactant. Toxic effects were observed at concentrations of ≥ 100 ug/plate. At 500 ug/plate the chemical was fatal to the test strains.
Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf

(100)

Type : Ames test
System of testing : Salmonella typhimurium
Concentration : 4, 20, 100, 500 and 2500 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: Henkel-method "Salmonella typhimurium reverse mutation assay"
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4
Remark : The test sample was suspended in water using Tween 80 as surfactant. Toxic effects were observed at concentrations of ≥ 100 ug/plate. At 500 ug/plate the chemical was fatal to the test strains.
Source : Henkel KGaA Duesseldorf

(101)

Type : Ames test
System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Concentration : 0.01-50 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: modified Ames test
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA Duesseldorf
 Henkel KGaA Duesseldorf
Test substance : Dodecanol, 90% purity, from Wako Pure Chemicals was tested.

(102)

Type : Ames test
System of testing : Salmonella typhimurium TA98, TA100, TA1535, TA1537, TA1538
Concentration : 0.01, 0.05, 0.1, 0.5, 1, 5, 10, 50 ug/plate
Cycotoxic conc. :
Metabolic activation : with and without
Result : negative
Method : other: modified Ames test
Year :
GLP : no data

5. Toxicity

Id 112-53-8

Date 05.11.2001

Test substance : as prescribed by 1.1 - 1.4
Source : Henkel KGaA Duesseldorf
Test substance : Dodecanol, 90% purity, from Wako Pure Chemicals was tested.

(103)

5.6 GENETIC TOXICITY 'IN VITRO'

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : other: albino mice, CFW 1
Route of admin. : gavage
Exposure period : 24, 48, and 72 hours
Doses : 5000 mg/kg body weight
Result :
Method : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : No statistically significant enhanced mean values of micronucleated cells in polychromatic erythrocytes were seen following oral doses of 5000 mg/kg body weight. No reduction in the ratio of polychromatic to normochromatic erythrocytes was seen.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(104)

Type : Micronucleus assay
Species : mouse
Sex : male/female
Strain : other: albino mice, CFW 1
Route of admin. : gavage
Exposure period : 24, 48, and 72 hours
Doses : 5000 mg/kg body weight
Result :
Method : OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : No statistically significant enhanced mean values of micronucleated cells in polychromatic erythrocytes were seen following oral doses of 5000 mg/kg body weight. No reduction in the ratio of polychromatic to normochromatic erythrocytes was seen.
Source : Henkel KGaA Duesseldorf

(105)

5.7 CARCINOGENITY

Species : mouse
Sex : female
Strain : Swiss
Route of admin. : dermal
Exposure period : 60 weeks
Frequency of treatment : 3 x / week
Post. obs. period : no

5. Toxicity

Id 112-53-8

Date 05.11.2001

Doses : After an initial dose of benz(a)anthracene, 20 µl of a mixture of 20 g Dodecanol in 100 ml Cyclohexanol per application.

Result :

Control group : no

Method : other: method not specified

Year :

GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Remark : Repeated skin application of dodecanol showed a probable weak activity in promoting skin tumors in female mice that had received an initiating dose of 7,12-dimethyl-benz(a)anthracene. The authors stated that the initiation dose of PAH alone is non-carcinogenic. After treatment with dodecanol there were two tumor bearing mice out of 30 initiated animals. The tumors appeared at 39 and 49 weeks. The topical application was moderate irritant.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(106)

Species : mouse

Sex : female

Strain : ICR

Route of admin. : dermal

Exposure period : 440 days

Frequency of treatment : 3 x week

Post. obs. period :

Doses : 10 mg/animal/application

Result :

Control group : other: with and without PAH induction

Method : other: method not specified

Year :

GLP : no data

Test substance : as prescribed by 1.1 - 1.4

Remark : The conclusion of the authors seems to be farfetched with respect to the fact of almost identical tumor incidences in the B[a]P plus Dodecanol and the B[a]P only treated groups.

Result : No tumors were observed in the 50 mice receiving dodecanol. Of the animals receiving dodecanol and B[a]P, 27 papillomas occurred in a total of 21 animals, 13 mice with squamous cell carcinoma. In a control group treated with B[a]P alone, 26 papillomas were observed in 16 animals, 12 of these tumors being squamous cell carcinoma. The authors conclude that these results suggest a weak to moderate co-carcinogenic effect.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(107)

Species : mouse

Sex : male/female

Strain : other: A/He

Route of admin. : i.p.

Exposure period : 8 weeks

Frequency of treatment : 3 injections/week

Post. obs. period : 16 weeks

Doses : Total doses of 2.4 g/kg and of 12 g/kg were given.

Result :

Control group : yes

Method : other: Test for Carcinogenicity by Pulmonary Tumor Response

5. Toxicity

Id 112-53-8

Date 05.11.2001

Year : 1973
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Result : Lung tumors were observed in 2/15 female mice in the high dose group, and in 2/15 males and in 3/13 females in the low dose group. The lung tumor rate was not statistically significant relative to either untreated or vehicle controls. No tumors were found in other organs examined.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : Dodecanol was administered in 0.1 ml tricaprylin.

(108)

5.8 TOXICITY TO REPRODUCTION

Type : One generation study
Species : rat
Sex : male/female
Strain : Wistar
Route of admin. : oral feed
Exposure period : 14 days
Frequency of treatment : permanent by diet
Premating exposure period
Male : 14 days
Female : 14 days
Duration of test : 5 weeks
Doses : 0, 100, 500, 2000 mg/kg bw/day
Control group : yes
NOAEL Parental : = 2000 mg/kg bw
NOAEL F1 Offspr. : = 2000 - mg/kg bw
Method : other: Combined Repeat Dose and Reproductive/Developmental Toxicity Screening Test
Year :
GLP : yes
Test substance : as prescribed by 1.1 - 1.4
Result : No effects were seen on reproductive or developmental parameters up to doses of 2000 mg/kg bw/day. 1-Dodecanol in the doses administered had no influence on body weight, weight gain, food consumption and food efficiency in the parental generation. Pregnancy rates were not statistically altered and there were no differences in the lengths of the gestation periods. No organ toxicity was observed in the females. There was no effect on the number of pups per litter, weight, sex ratio or mortality rate from days 1-5 after birth. Autopsy indicated no effect from 1-Dodecanol under the conditions of this experiment.
Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf
Test substance : 99% Dodecanol from Sigma (# L 5375) was tested.

(109)

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.10 OTHER RELEVANT INFORMATION

5. Toxicity

Id 112-53-8
Date 05.11.2001

Type : Metabolism
Source : Henkel KGaA Duesseldorf

(110) (111) (112)

5.11 EXPERIENCE WITH HUMAN EXPOSURE

Remark : 51 subjects allergic to wool wax alcohols have been tested, according to the ICDRG-method (305 in vaseline). Scores were measured after 24, 48 and 72 h. 1-Dodecanol reacted in 9 cases with reaction grade ++ (Erytheme and Papeln or Infiltrate) and +++ (erytheme, infiltrate or rather papulovesicle). The authors conclude that free fatty alcohols and especially 1-Dodecanol play a major part with respect to allergic reactions caused by wool wax in subjects allergic to wool wax.

Source : Henkel KGaA Duesseldorf
Henkel KGaA Duesseldorf

(113)

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7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

7.3 RISK ASSESSMENT